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SPECTRAL ANALYSIS OF METRIC GRAPHS WITH INFINITE RAYS

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Abstract. We conduct a detailed analysis for finite metric graphs that have a semi-infinite chain (a ray) attached to each vertex. We show that the adjacency matrix of such a graph gives rise to a selfadjoint operator that is unitary equivalent to a direct sum of a finite number of simplest Jacobi matrices. This permitted to describe spectrums of such operators and to explicitly construct an eigenvector decomposition.

1. Introduction

Spectral theory of graphs is one of most topical research directions in modern mathematical physics, see [1]–[8] and the references therein. This is due to both the problems pertaining to the theory itself and the solution of particular problems that arise in the theory of information, communication, power, and transportation networks.

The simplest nonoriented graph G is a pair (V, E), where V is a nonempty set, the set of vertices, and E is a set of edges that join vertices in V. There is an adjacency matrix $A(G) = (a_{ij})_{i,j=1}^{|V|}$ connected with the graph G, with the elements a_{ij} equal 1 if the vertices with the indices i and j are joined with an edge, and equal 0 if no such edge exists. If each edge is supplied with length, then the graph is called metric. The adjacency matrix of such a graph has the matrix element a_{ij} equal to the length of the edge that joins the vertices i and j, and zero otherwise.

If the graph is countable, then the matrix $A(G)$ gives rise to a selfadjoint operator $\mathbb{A}$ on the Hilbert space $l_2(V)$ such that its spectrum could have a discrete, $\sigma_p(\mathbb{A})$, and a continuous, $\sigma_c(\mathbb{A})$, components. Spectral analysis of a graph G means spectral analysis of the selfadjoint operator $\mathbb{A}$ on the Hilbert space $l_2(V)$.

Spectral analysis of finite graphs reduces to spectral analysis of nonnegative symmetric finite matrices, and it is now a well developed part of graph theory [2]. There is also spectral theory constructed for some countable graphs [9, 10].

The most simple infinite graph $A_{\mathbb{N}}$ is a half-bounded chain having its vertices indexed with natural numbers, $\mathbb{N} = \{1, 2, \dots\}$, and its edges join only the vertices that have consecutive indices. The length of all such edge equals 1.

Such a graph will be called a ray.

The adjacency matrix of a half-bounded chain $A_{\mathbb{N}}$ is a Jacobi matrix J_0 with zeros on the main diagonal and ones on the adjacent diagonals. It is well known that the matrix J_0 gives rise to a selfadjoint operator on the space $l_2(\mathbb{N})$, whose spectrum is simple, pure continuous, and coincides with the line segment $[-2, 2]$, see [4, 13, 12]. Moreover, the operator J_0 on the space $l_2(\mathbb{N})$ is subject to a spectral theorem on decomposition with respect to generalized eigenfunctions, see [13]. For $\lambda \in [-2, 2]$, the vector-valued

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function $\varphi(\lambda) = (\varphi_1(\lambda), \varphi_2(\lambda), \ldots)$, where $\varphi_j(\lambda) = P_j(\lambda), j \geq 0$, is a generalized eigenfunction for the operator J_0 and corresponds to the eigenvalue λ, that is, $J_0\varphi(\lambda) = \lambda\varphi(\lambda)$. Here $P_j(\lambda)$ is a polynomial in λ of degree j. It can be expressed as $P_j(\lambda) = U_j(\frac{\lambda}{2})$ in terms of the second kind Chebyshev polynomials $U_j(z) = \frac{\sin((j+1)\arccos z)}{\sin(\arccos z)}$. The polynomials $P_j(\lambda)$ satisfy the recurrence relation $P_{j+1}(\lambda) = \lambda P_j(\lambda) - P_{j-1}(\lambda)$ with the initial conditions $P_{-1}(\lambda) = 0,\ P_0(\lambda) = 1,\ P_1(\lambda) = \lambda$.

To every vector $x \in l_2(\mathbb{N})$ there is a corresponding Fourier transform $\widetilde{x}(\lambda)$ with respect to generalized eigenvectors,

$$\widetilde{x}(\lambda) \equiv \mathfrak{F}x = (x, \varphi(\lambda))_{l_2} = \sum_{j=1}^{\infty} x_j \varphi_j(\lambda). \tag{1}$$

The function $\widetilde{x}(\lambda)$ belongs to the space $L_2([-2,2], \rho(\lambda)d\lambda) \equiv L_2(\rho)$ of square integrable functions on the line segment $[-2,2]$ with the weight $\rho(\lambda) = \frac{1}{2\pi}\sqrt{4-\lambda^2} \equiv \rho_0(\lambda)$.

The inverse Fourier transform is also defined on the whole space $L_2(\rho)$,

$$x \equiv \mathfrak{F}^{-1}\widetilde{x} = \int_{-2}^{2} \widetilde{x}(\lambda)\varphi(\lambda)\rho(\lambda)\,d\lambda. \tag{2}$$

The following Parseval identity holds for arbitrary $x, y \in l_2(\mathbb{N})$:

$$(x, y)_{l_2} = (\widetilde{x}, \widetilde{y})_{L_2(\rho)}. \tag{3}$$

It was shown in [10] that a spectral analysis of countable graphs that are formed from a finite graph by adjoining a single ray can be carried out using Jacobi matrices that have only a finite number of elements different from the corresponding elements of the Jacobi matrix J_0. This permitted in [9, 10] to obtain explicit formulas in the cases of star, complete, and cyclic graphs, as well as for some other types of graphs.

The paper [11] deals with spectral properties of countable graphs that are formed from finite graphs by adjoining infinite rays to some vertices. It is shown that the adjacency matrix of such graphs is unitary equivalent to an orthogonal sum of a finite symmetric matrix and several special Jacobi matrices that have not more than four elements different from the corresponding ones in the simplest Jacobi matrix J_0. This permits to carry out a complete and explicit analysis of such graphs.

The purpose of this research is to carry out a spectral analysis in an explicit form for metric graphs that have semibounded rays attached to every vertex.

2. Spectral analysis of simplest Jacobi matrices

The simplest Jacobi matrices are the matrices J that have only a finite number of elements different from the corresponding elements of the Jacobi matrix J_0. Spectral theorem for such matrices can be explicitly stated, see [9, 10, 11, 12, 13]. Let us formulate the result regarding the matrices J_a^b of the form

$$J_a^b = \begin{vmatrix} b & a & 0 & 0 & \ldots \\ a & 0 & 1 & 0 & \ldots \\ 0 & 1 & 0 & 1 & \ldots \\ 0 & 0 & 1 & 0 & \ldots \\ & \ldots & \ldots & & \end{vmatrix} \tag{4}$$

Theorem 1. *A Jacobi matrix J_b^a of the form (4) gives rise a bounded selfadjoint operator on the space $l_2(\mathbb{N})$ such that its spectrum consists of a simple absolutely continuous component, which is the line segment $[-2,2]$, and at most two eigenvalues λ that are zeros of the spectral polynomial*

$$p(\lambda) = a^4 + b^2 + b(a^2-2)\lambda - (a^2-1)\lambda^2, \tag{5}$$

satisfying the condition that the absolute value of the number $\mu = \frac{\lambda - b}{a^2}$ is less than 1.

A necessary and sufficient condition for the matrix J_b^a *to have*

1) *two eigenvalues is the condition that* $a^2 > 2,\ |b| < a^2 - 2$*;*
2) *a single eigenvalue is the condition that* $|b| \geq a^2 - 2$*, and then* $\operatorname{sign}\lambda = \operatorname{sign} b$*;*
3) *no eigenvalues is the condition* $a^2 \leq 2,\ |b| \leq 2 - a^2$*.*

To every eigenvalue $\lambda = \mu + \mu^{-1}$ *there is a corresponding eigenvector in the space* $l_2(\mathbb{N})$*,*

$$e_\mu = (a^{-1}, \mu, \mu^2, \mu^3, \ldots, \mu^j, \ldots)\,. \tag{6}$$

Also, to every $\lambda \in [-2, 2]$ *there is a generalized eigenvector,*

$$\begin{aligned}\varphi(\lambda) = (a, P_1(\lambda) - bP_0(\lambda), P_2(\lambda) &- bP_1(\lambda) - (a^2-1)P_0(\lambda),\\ &\ldots, P_{j-1}(\lambda) - bP_{j-2}(\lambda) - (a^2-1)P_{j-3}(\lambda), \ldots).\end{aligned} \tag{7}$$

A decomposition with respect to the given eigenvector-valued functions and the Parseval identity with the spectral density $\rho(\lambda) = \frac{\sqrt{4-\lambda^2}}{2\pi p(\lambda)}$ *on the absolutely continuous part of the spectrum hold true.*

Corollary. (1) *If* $a = 1$*, the matrix* J_b *will have a single eigenvalue,* $\lambda = b + b^{-1}$*, if and only if* $|b| > 1$*.*

(2) *If* $b = 0$*, the matrix* J^a *will have two eigenvalues,* $\lambda = \pm a^2(a^2-1)^{-1/2}$*, if and only if* $a > \sqrt{2}$*. If* $a \leq \sqrt{2}$*, it has no eigenvalues.*

The following result will be used in the sequel.

Theorem 2. *For the Hilbert space* $H = l_2(\mathbb{N}) \oplus l_2(\mathbb{N})$*, the orthogonal sum* $J_b \oplus J_{-b}$ *of Jacobi matrices is unitary equivalent to the orthogonal sum* $J^a \oplus J_0$*, where* $a = \sqrt{1+b^2}$ *and* b *is an arbitrary real number.*

Proof. Let $A = J_b \oplus J_{-b}$ and $\{e_k\}_{k=1}^\infty$ be a standard basis in the subspace $l_2(\mathbb{N}) \oplus \{0\}$ of the space H, and $\{e_{-k}\}_{k=1}^\infty$ be a standard basis in the subspace $\{0\} \oplus l_2(\mathbb{N})$, the subspaces where the matrices J_b and J_{-b} act. Then

$$Ae_{\pm 1} = \pm b e_{\pm 1} + e_{\pm 2}, \quad Ae_{\pm k} = e_{\pm(k-1)} + e_{\pm(k+1)}, \quad k \geq 2. \tag{8}$$

In the space H, consider a new basis $\{\widehat{e}_{\pm k}\}_{k\in\mathbb{N}}$, which is related to the initial basis $\{e_{\pm k}\}_{k\in\mathbb{N}}$ via the identities $\widehat{e}_1 = \frac{1}{\sqrt{2}}(e_1 + e_{-1})$, $\widehat{e}_n = \frac{1}{a\sqrt{2}}(b(e_{n-1} + e_{-(n-1)}) + e_n + e_{-n})$, $n \geq 2$, where $a = \sqrt{1+b^2} > 0$ and $\widehat{e}_{-n} = \frac{1}{a\sqrt{2}}(e_n - e_{-n} - b(e_{n+1} + e_{-(n+1)}))$, $n \geq 1$. It is easy to see that, on the space H_1 with the basis $\{\widehat{e}_k\}_{k\in\mathbb{N}}$, the operator A acts as the Jacobi matrix J^a, and, on the space H_{-1}, the operator A acts as the Jacobi matrix J^0.

To finish the proof of the theorem, it only remains to show that $H_1 \perp H_{-1}$ and $H = H_1 \oplus H_{-1}$. This can be easily done by using an explicit form of the new basis and the action of the operator A given by (8) with respect to the constructed basis. Thus the matrix of the operator A, with respect to the new basis, has the form $A = J^a \oplus J_0$. □

3. Metric graphs with attached rays

Let $G(n,\infty)$ be a countable graph that is obtained from the connected metric graph $G(n)$ with n vertices by attaching, to each vertex of the graph, a ray that is a semi-bounded chain. All vertices of a ray are indexed with integers written in the lower index whereas the vertices of the graph $G(n)$ are indicated as an upper index. Hence, all vertices V of the graph $G(n,\infty)$ are vertices of n rays and have two indices, the upper index is $j = 1, \ldots, n$ that is the index of the ray, and the lower index $i \in \mathbb{N}$ that is the number i of the vertex on the j-th ray. The adjacency matrix of the graph $G(n,\infty)$ gives rise to a bounded selfadjoint operator $\mathbb{A}$ on the Hilbert space $l_2(\mathbb{N})$, acting by

$$(9)\qquad \begin{aligned} (\mathbb{A}x)_1^j &= \sum_{k=1}^{n} a_{jk} x_1^k + x_2^j, \\ (\mathbb{A}x)_i^j &= x_{i-1}^j + x_{i+1}^j, \quad i \geq 2, \quad j = 1, \ldots, n. \end{aligned}$$

Here the components of the vectors x and $\mathbb{A}x$ of the space $l_2(V)$, which correspond to the i-th vertex on the j-th ray, are denoted with the upper index j and the lower index i. The matrix $\|a_{j,k}\|_{j,k=1}^n = A$ is the adjacency matrix of the metric graph $G(n)$. The main result is given by the following theorem.

Theorem 3. *Let $\{\lambda_j\}_{j=1}^n$ be all eigenvalues of the adjacency matrix A of the metric graph $G(n)$, counting multiplicities.*

Then the operator $\mathbb{A}$, which is selfadjoint on the space $l_2(V)$ and corresponds to the graph $G(n,\infty)$ with rays attached to each vertex of the metric graph $G(n)$, is unitary equivalent to the orthogonal sum $\oplus_{k=1}^n J_{\lambda_k}$ of Jacobi matrices J_{λ_k} that have the numbers $\lambda_k, 0, 0, \ldots$ on the main diagonals and the numbers $1, 1, \ldots$ on the adjacent diagonals, that is, there exists a unitary operator U on the space $l_2(V)$ such that

$$(10)\qquad U\mathbb{A}U^{-1} = \oplus_{k=1}^n J_{\lambda_k}.$$

Proof. Let $\{e_i^j\}_{j=1,\, i\in\mathbb{N}}^n$ be a standard basis in the space $l_2(V)$, corresponding to the above indexing of the vertices V of the graph $G(n,\infty)$. By (9), the operator $\mathbb{A}$ acts on vectors of the standard basis by

$$(11)\qquad \begin{aligned} \mathbb{A}e_1^j &= \sum_{k=1}^{n} a_{jk} e_1^k + e_2^j, \\ \mathbb{A}e_i^j &= e_{i-1}^j + e_{i+1}^j, \quad i \geq 2. \end{aligned}$$

In the space E^n, consider an orthonormal system of eigenvectors $\{e_k\}_{k=1}^n$ of the symmetric matrix $A = \|a_{i,l}\|_{i,l=1}^n$, corresponding to the eigenvalues $\{\lambda_k\}_{k=1}^n$. The components $e_{k,j}$ of the eigenvalues $e_k = \operatorname{col}(e_{k,1}, \ldots, e_{k,n})$ form a unitary matrix $U = \|u_{k,j}\|_{k,j=1}^n$, $u_{k,j} \equiv e_{k,j}$, in the Euclidean space E^n. Construct a new orthonormal basis $\{\widehat{e}_i^j\}_{j=1,\, i\in\mathbb{N}}^n$ in the space $l_2(V)$ by setting

$$(12)\qquad \widehat{e}_i^j = \sum_{k=1}^{n} u_{j,k} e_i^k.$$

Then the operator $\mathbb{A}$ acts as the Jacobi matrix J_{λ_j} on the subspaces $H^j \subset l_2(V)$ with the basis$\{\widehat{e}_i^j\}_{i\in\mathbb{N}}$. Indeed,

$$\mathbb{A}\widehat{e}_1^j = \sum_{k=1}^{n} u_{jk}\mathbb{A}e_1^k = \sum_{k=1}^{n} u_{jk}\left(\sum_{\alpha=1}^{n} a_{k\alpha}e_1^\alpha + e_2^k\right) = \lambda_j \sum_{\alpha=1}^{n} u_{j\alpha}e_1^\alpha + \sum_{\alpha=1}^{n} u_{j\alpha}e_2^\alpha = \lambda_j \widehat{e}_1^j + \widehat{e}_2^j,$$

and, for $i \geq 2$,

$$\mathbb{A}\widehat{e}_i^j = \widehat{e}_{i-1}^j + \widehat{e}_{i+1}^j.$$

Then the unitary operator $\mathbb{U}$ that maps the initial basis $\{e_i^j\}$ into the new one, $\{\widehat{e}_i^j\}$, satisfies the claim of the theorem. □

4. Examples

4.1. A star graph with infinite rays.

Proposition 1. *Let $S(n,\infty)$ be a star graph with n infinite rays. Then its adjacency matrix gives rise to a selfadjoint operator that is unitary equivalent to an orthogonal sum of the Jacobi matrices,* $J^{\sqrt{n}} \oplus \underbrace{J_0 \oplus \cdots \oplus J_0}_{n-1}$.

Proof. The graph $S(n,\infty)$ can be considered as the finite star graph $S(n-1)$ with a single vertex, the center, and $n-1$ edges coming out of the vertex, together with infinite rays attached to each vertex of the graph. Since the star graph $S(n-1)$ has the eigenvalues $\lambda_0 = 0$ of multiplicity $n-1$ and $\lambda_\pm = \pm\sqrt{n-1}$ [1, 2], the proof follows from Theorems 2 and 3. □

4.2. **A complete graph with infinite rays.**

Proposition 2. *Let $K(n,\infty;d)$ be a complete graph with n vertices each pair of which is joined with an edge of length d, and such that an infinite ray is attached to each of the n vertices. Then its adjacency matrix gives rise to a selfadjoint operator that is unitary equivalent to an orthogonal sum of Jacobi matrices,* $J_{(n-1)d} \oplus \underbrace{J_{-d} \oplus \cdots \oplus J_{-d}}_{n-1}$.

Proof. It is known [1, 2] that eigenvalues of a complete graph with n vertices are the numbers $\lambda = -d$ of multiplicities $n-1$, and $\lambda = (n-1)d$. Then the claim follows from Theorem 3. □

Theorem 1 gives a description of eigenvalues. If $d > 1$, then the adjacency matrix of the graph $K(n,\infty;d)$ has n eigenvalues, $\lambda_1 = (n-1)d + ((n-1)d)^{-1}$, and $\lambda_j = -d - d^{-1}$, $j = 2,\ldots,n$. If $(n-1)^{-1} < d \le 1$, then the adjacency matrix of the graph $K(n,\infty;d)$ has a unique eigenvalue, λ_1. If $d \le (n-1)^{-1}$, then the matrix of the graph $K(n,\infty;d)$ has no eigenvalues.

4.3. **A double star graph with rays attached.**

Proposition 3. *Let $S(p,\infty;q,\infty,d)$ be a double star graph that consists of two star graphs with infinite rays $S(p,\infty)$ and $S(q,\infty)$ and the centers joined with an edge of length d. Then the adjacency matrix of such a double star graph is unitary equivalent to an orthogonal sum of the matrices J^{a_+} and J^{a_-}, and $p+q-2$ matrices J_0. Here $a_\pm = \sqrt{1+\lambda_\pm}$, where $\lambda_\pm = \frac{1}{2}(p+q+d^2-2 \pm \sqrt{(p+q+d^2-2)^2 - 4(p-1)(q-1)})$.*

Proof. The graph $S(p,\infty;q,\infty,d)$ can be obtained by attaching an infinite ray to each vertex of the finite metric graph $S(p-1,q-1;d)$ that consists of two star graphs with, correspondingly, $p-1$ and $q-1$ edges of length 1 and the centers joined with an edge of length d. It is easy to see that the characteristic polynomial of the adjacency matrix of the graph $S(p-1,q-1;d)$ can be written as $\lambda^{p+q-4}(\lambda^4 - (p+q+d^2-4)\lambda^2 + (p-1)(q-1))$. Hence, spectrum of the graph $S(p-1,q-1;d)$ has $\lambda = 0$ with multiplicity $p+q-4$ and four more zeros of the polynomial $\lambda^4 - (p+q+d^2-4)\lambda^2 + (p-1)(q-1))$. Then Proposition 3 follows from Theorems 2 and 3. Using Theorem 1 we conclude that the double star graph $S(p,\infty;q,\infty,d)$ with $p,q \ge 2$ will have two eigenvalues for $p = 2$ or $q = 2$, as well as for $p,q \ge 3$, if $d^2 \ge pq - 2p - 2q + 4$. In all other cases, the double star graph has 4 eigenvalues. □

4.4. **A cyclic graph with attached rays.**

Proposition 4. *Let $C(n,\infty)$ be a cyclic graph with n vertices and with a ray attached to each one. Then the adjacency matrix of the graph $C(n,\infty)$ is unitary equivalent to an orthogonal sum of Jacobi matrices, $\oplus_{k=1}^{n} J_{\lambda_k}$, where $\lambda_k = 2\cos\frac{2k\pi}{n}$, $k = 0,\ldots,n-1$.*

Proof. The proof follows from Theorem 3, since the eigenvalues for the cyclic graphs $C(n)$ with n vertices are given by $\lambda_k = 2\cos\frac{2k\pi}{n}$, $k = 0,\ldots,n-1$. [1, 2] □

Let us note that the eigenvalues can be paired, λ_k and $\lambda_{m-k} = -\lambda_k$, if $n = 2m$. Hence, using Theorem 2 and an explicit form of the eigenvalues, there is a unitary equivalence obtained in [11] for the adjacency matrices A_n of the graphs $C(n, \infty)$ with the Jacobi matrices

$$\begin{aligned}
&J^{\sqrt{5}} \oplus J_0 \oplus J_0 \oplus J_0, \quad \text{if} \quad n = 4,\\
&J^{\sqrt{5}} \oplus J^{\sqrt{2}} \oplus J^{\sqrt{2}} \oplus J_0 \oplus J_0 \oplus J_0, \quad \text{if} \quad n = 6,\\
&J^{\sqrt{5}} \oplus J^{\sqrt{3}} \oplus J^{\sqrt{3}} \oplus \underbrace{J_0 \oplus \ldots \oplus J_0}_{5}, \quad \text{if} \quad n = 8,\\
&J^{\sqrt{5}} \oplus J^{2} \oplus J^{2} \oplus J^{\sqrt{2}} \oplus J^{\sqrt{2}} \oplus \underbrace{J_0 \oplus \ldots \oplus J_0}_{7}, \quad \text{if} \quad n = 12.
\end{aligned}$$

4.5. **A finite chain with a ray attached to each vertex.**

Proposition 5. *Let $A(n, \infty)$ be a finite chain of n vertices with an infinite chain attached to each one. Then the adjacency matrix of the graph $A(n, \infty)$ is unitary equivalent to the orthogonal sum $\oplus_{k=1}^n J_{\lambda_k}$ of Jacobi matrices, where $\lambda_k = 2\cos\frac{k\pi}{n+1}$, $k = 1, \ldots, n$.*

Proof. The proof follows from Theorem 3 and a use of known eigenvalues of a finite chain [1, 2]. □

Let us note that, by using Theorem 1, one can give an explicit description of the spectrum and the eigenvector decomposition corresponding to the discrete and continuous parts of the spectrum for the graphs considered in Propositions 1–5.

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