LIETUVOS MATEMATIKOS RINKINYS
Proc. of the Lithuanian Mathematical Society, Ser. A
Vol. 61, 2020, pages 1–6
https://doi.org/10.15388/LMR.2020.22474

Relations between spectrum curves of discrete Sturm–Liouville problem with nonlocal boundary conditions and graph theory

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Received December 1, 2020; published online February 18, 2021

Abstract. Sturm–Liouville problem with nonlocal boundary conditions arises in many scientific fields such as chemistry, physics, or biology. There could be found some references to graph theory in a discrete Sturm–Liouville problem, especially in investigation of spectrum curves. In this paper, relations between discrete Sturm–Liouville problem with nonlocal boundary conditions characteristics (poles, critical points, spectrum curves) and graphs characteristics (vertices, edges and faces) were found.

Keywords: Sturm–Liouville problem; spectrum curves; nonlocal boundary conditions; graphs

AMS Subject Classification: 34B24; 05C10

1 A discrete Sturm–Liouville Problem

In this paper, particular properties of the spectrum of *a discrete Sturm–Liouville Problem* (dSLP) [1, 5, 6] with *Nonlocal Boundary Conditions* (NBCs) were found using Euler's charakteristic formula [4].

We introduce a uniform grid and we use notation $\bar{\omega}^h = \{t_j = jh, j = 0, \ldots, n; nh = 1\}$ for $2 < n \in \mathbb{N}$, and $\mathbb{N}^h := (0, n) \cap \mathbb{N}$, $\overline{\mathbb{N}}^h = \mathbb{N}^h \cup \{0, n\}$. Also, we make an assumption that ξ is located on the grid, i.e., $\xi = mh = m/n$, $0 < m < n$. We denote $\mathbb{N}_o = \{k \in \mathbb{N} \colon k - \text{odd}\}$, $\mathbb{N}_e = \{k \in \mathbb{N} \colon k - \text{even}\}$.

Let us consider a dSLP (an approximation by Finite-Difference Scheme)

$$\frac{U_{i+1} - 2U_i + U_{i-1}}{h^2} = \lambda U_i, \quad i = 1, \ldots, n-1, \tag{1}$$

Table 1. Functions $Z^h(q)$ and $P^h_\xi(q)$.

Case	$Z^h(q)$	$P^h_\xi(q)$
a)	$\sin(\pi q)\pi^{-1}q^{-1}(1-hq)^{-1}$	$\sin(\xi\pi q)\pi^{-1}q^{-1}(1-hq)^{-1}$
b)	$\sin(\pi q)h\sin^{-1}(\pi qh)$	$\cos(\xi\pi q)$
c)	$\cos\big(\pi q(1-h/2)\big)\cos^{-1}(\pi qh/2)$	$\cos\big(\pi q(\xi-h/2)\big)\cos^{-1}(\pi qh/2)$
d)	$-\cos\big(\pi q(1-h/2)\big)\cos^{-1}(\pi qh/2)$	$2\sin\big(\pi q(\xi-h/2)\big)\sin(\pi qh/2)h^{-1}$

$\lambda\in\mathbb{C}$ with classical discrete Dirichlet or Neumann Boundary Condition (BC)

$$U_0=0, \tag{2_d}$$
$$U_1=U_0 \tag{2_n}$$

and NBC:

$$U_n=\gamma U_m, \tag{3_0}$$
$$U_n=\gamma\frac{U_{m+1}-U_{m-1}}{2h}. \tag{3_1}$$

So, we have four cases of BCs: a) (2_d)–(3_0), b) (2_d)–(3_1), c) (2_n)–(3_0), d) (2_n)–(3_1). We denote $\varkappa=0$ for (3_0) BC and $\varkappa=1$ for (3_1) BC; $K:=\gcd(n,m)$ and $N:=n/K$, $M:=m/K$ in the case a), b), and $K:=\gcd(2n-1,2m-1)\in\mathbb{N}_o$ and $N:=\big((2n-1)/K+1\big)/2$, $M:=\big((2m-1)/K+1\big)/2$ in the case c).

Let us consider a bijection (see [2])

$$\lambda=\lambda^h(q):=\frac{4}{h^2}\sin\frac{\pi qh}{2} \tag{4}$$

between $\mathbb{C}_\lambda:=\mathbb{C}$ and $\mathbb{C}^h_q$, $\mathbb{C}^h_q:=\mathbb{R}^h_q\cup\mathbb{C}^{h+}_q\cup\mathbb{C}^{h-}_q$, $\mathbb{R}^h_q:=\mathbb{R}^-_y\cup\{0\}\cup\mathbb{R}^h_x\cup\{n\}\cup\mathbb{R}^{h+}_y$, $\mathbb{R}^-_y:=\{q=\imath y: y>0\}$, $\mathbb{R}^h_x:=\{q=x: 0<x<n\}$, $\mathbb{R}^{h+}_y:=\{q=n+\imath y: y>0\}$, $\mathbb{C}^{h+}_q:=\{q=x+\imath y: 0<x<n, y>0\}$, $\mathbb{C}^{h-}_q:=\{q=x+\imath y: 0<x<n, y<0\}$. The general solution U_j for a discrete equation (1) is equal to:

$$U_j=C_1\sin(\pi qt_j)(1-hq)^{-1}\pi^{-1}q^{-1}+C_2\cos(\pi qt_j).$$

Then by using BCs (2) and (3) we get an equation:

$$Z^h(q)=\gamma P^h_\xi(q),\quad q\in\mathbb{C}^h_q,$$

where functions $Z^h(q)$ and $P^h_\xi(q)$ are determined in Table 1.

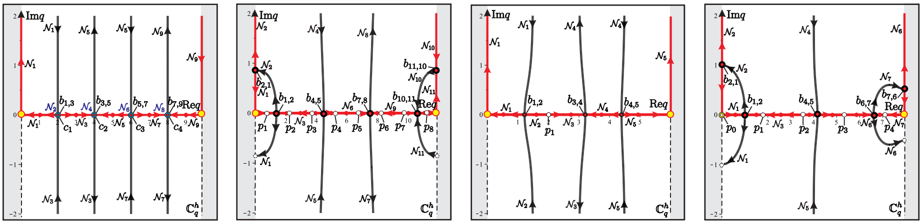
Constant eigenvalues. For any constant eigenvalue $\lambda\in\mathbb{C}_\lambda$ there exists the *Constant Eigenvalue Point* (CEP) $q\in\mathbb{C}_q$. CEP are roots of the system [2]:

$$Z^h(q)=0,\qquad P^h_\xi(q)=0.$$

For every CEP c_j we define *nonregular Spectrum Curve* $\mathcal{N}_j=\{c_j\}$.

Nonconstant eigenvalues. Let us consider *Complex Characteristic Function*:

$$\gamma_c(q)=\gamma_c(q;\xi):=\frac{Z^h(q)}{P^h_\xi(q)},\quad q\in\mathbb{C}^h_q. \tag{5}$$



(a) (b) (c) (d)

Fig. 1. Spectrum Curves [1].

All *nonconstant eigenvalues* (which depend on the parameter γ) are γ-points of (Complex-Real) *Characteristic Function* (CF)[7]. CF $\gamma(q)$ is the restriction of Complex CF $\gamma_c(q)$ on a set $\mathcal{D}_{\boldsymbol{\xi}} := \{q \in \mathbb{C}_q^h\colon \operatorname{Im}\gamma_c(q) = 0\}$. A set $\mathcal{E}_{\boldsymbol{\xi}}(\gamma_0) := \gamma^{-1}(\gamma_0)$ is the set of all nonconstant eigenvalue points for $\gamma_0 \in \mathbb{R}$. If $q \in \mathcal{D}_{\boldsymbol{\xi}}$ and $\gamma_c'(q) \neq 0$ (q is not a Critical Point (CP) of CF), then $\mathcal{E}_{\boldsymbol{\xi}}(\gamma)$ is smooth parametric curve $\mathcal{N}\colon \mathbb{R} \to \mathbb{C}_q^h$ locally and we can add arrow on this curve (arrows show the direction in which $\gamma \in \mathbb{R}$ is increasing). We call such curves *regular Spectrum Curves* [2]. The regular Spectrum Curves form Spectrum Domain in $\mathbb{C}_q^h \cup \{\infty\}$ (see Fig. 1).

Each regular Spectrum Curve begins at the pole point ($\gamma = -\infty$) of CF and ends at the pole point ($\gamma = +\infty$) of CF. We denote a set Poles $\mathcal{P} := \{p_i, i = \overline{1, n_p}\}$, where n_p is the number of poles at $\mathbb{C}_q^h$. For our problems $\mathcal{P} \subset \mathbb{R}_x^h \cup \{0\}$ and all poles are of the first order (we write $\deg^+(p) = 1$, $p \in \mathcal{P}$).

Two or more Spectrum Curves may intersect at CP. We denote a set CP $\mathcal{B} := \{b_i, i = \overline{1, n_b}\}$, where n_b is the number of CPs at $\mathbb{C}_q^h$. The number of CPs at $\mathbb{R}_q^h$ and $\mathbb{C}_q^{h+}$ we denote as n_{cr} and n_{cr}^+, respectively. Note that the part of the spectrum domain in set $\mathbb{C}_q^{h+}$ is symmetric to the part in set $\mathbb{C}_q^{h-}$. So, $n_b = n_{cr} + 2n_{cr}^+$. If $b \in \mathcal{B}$ then $\deg^+(b)$ is one unit larger than the order of CP b.

The pole at $q = \infty$ is of

$$n_\infty = n - m - \varkappa \tag{6}$$

order. For (3_1) BC ($\varkappa = 1$) in the case $n = m + 1$ the point $q = \infty$ is CP of the first order. So, $n_\infty^+ = \deg^+(\infty) = n_\infty + 2\varkappa\lfloor(m+1)/n\rfloor$. A number of all CPs is $\tilde{n}_b = n_b + \varkappa\lfloor(m+1)/n\rfloor$.

For poles and CP $\deg^+(q)$, $q \in \mathcal{P} \cup \mathcal{B} \cup \{\infty\}$, corresponds to the number of outgoing Spectrum Curves at that point. Note that incoming Spectrum Curves alternate with outgoing, so $\deg^+(q) = \deg^-(q)$.

2 Graphs. Euler's characteristic. Digraphs

A graph is a pair of sets $G = (V, E)$ that consists of a non-empty set of vertices (nodes or points), $V = \{v_i, \overline{i = 1, I}, I \in \mathbb{N}\}$ and a set of edges $E = \{e_i, \overline{i = 1, J}, J \in \mathbb{N}\}$. We say that $e_j := (v_{i_1}, v_{i_2}) =: v_{i_1}v_{i_2} = v_{i_2}v_{i_1} \in E$, $v_{i_1}, v_{i_2} \in V$, and v_{i_1} (or v_{i_2}) is the end of an edge e_j. The powers of sets V and E are $|V| = v$ and $|E| = e$. The *faces* of a planar graph are the areas which are surrounded by edges. We denote f the number of such faces.

The Euler's characteristic χ of a subdivision of a surface is $\chi = v - e + f$. Since spectrum curves are on Riemann's sphere $\bar{\mathbb{C}} = \mathbb{C} \cup \infty$, we are interested in Euler's characteristic of a sphere S^2. *Euler's characteristics of a plane* [4] *of and a sphere* [3] *are* $\chi = 2$.

In graph theory, a directed graph or *digraph* is a graph that is made up of a set of points connected by arrows (edges with direction). For a vertex, the number of head ends adjacent to a vertex is called the indegree of the vertex and the number of tail ends adjacent to a vertex is its outdegree. Let $G = (V, A)$ and $v \in V$. The indegree of v is denoted $\deg^-(v)$ and its outdegree is denoted $\deg^+(v)$. If for every vertex $v \in V$, $\deg^+(v) = \deg^-(v)$, the graph is called a balanced digraph. Simple digraphs have no loops and no multiple arrows with same source and target points. The degree sum formula states that, for a digraph,

$$\sum_{v\in V} \deg^-(v) = \sum_{v\in V} \deg^+(v) = |A| = e. \tag{7}$$

The ordered pair is called weakly connected if an undirected path leads from v_1 to v_2 after replacing all of its directed arrows with undirected edges.

3 Relations between dSLP and graphs properties

It is possible to define relations between properties of dSLP and graph theory. Poles or CPs refer to vertices of a certain graph and parts of Spectrum Curves could be interpreted as edges. In our case, we have a simple balanced weakly connected digraph.

3.1 Properties of Spectrum Curves

Poles, CPs, regular and nonregular Spectrum Curves, CEPs were found by Bingelė [1].

There is $n-1$ Spectrum Curves for every $n \in \mathbb{N}$, $n \geq 2$. Nonregular Spectrum Curves are CEPs and belong to $\mathbb{R}_x^h = (0, n)$. The number of such Spectrum Curves is equal to

$$n_{ce} = K - 1, \tag{8_a}$$
$$n_{ce} = K \quad \text{for } N \in \mathbb{N}_e, \qquad n_{ce} = 0 \quad \text{for } N \in \mathbb{N}_o, \tag{8_b}$$
$$n_{ce} = (K-1)/2, \tag{8_c}$$
$$n_{ce} = 0. \tag{8_d}$$

Number of regular Spectrum Curves $n_{nce} = n - 1 - n_{ce}$. The poles of CF belong to $\mathbb{R}_x^h \cup \{0\} \cup \{\infty\}$ and $n_p + n_\infty = n_{nce}$. So, we have formula

$$n_p + n_{ce} = m - 1 + \varkappa. \tag{9}$$

Let us denote

$$\deg_r^+ := \sum_{b\in\mathcal{B}\cap\mathbb{R}_q^h} \deg^+(b), \qquad \deg_c^+ := \sum_{b\in\mathcal{B}\cap\mathbb{C}_q^{h\pm}} \deg^+(b) = 2\sum_{b\in\mathcal{B}\cap\mathbb{C}_q^{h+}} \deg^+(b).$$

Let n_c is the number of Spectrum Curves parts in $\mathbb{C}_q^{h+}$ between two CP (including $q=\infty$ for $n=m+1$).

3.2 Spectrum domain as a graph

We consider Spectrum domain as graph on sphere (Riemann sphere $\bar{\mathbb{C}}$) because $\mathbb{C}_q^h \sim S^2$. The poles and CPs of the CF are the vertices of this graph. The point ∞ is the pole or CP.

Lemma 1. *The number of vertices is*

$$v = n_p + n_b + 1 = n_p + n_{cr} + 2n_{cr}^+ + 1. \tag{10}$$

From (7) we have $e = \sum_{p\in\mathcal{P}} \deg^+(p) + \sum_{b\in\mathcal{B}} \deg^+(b) + \deg^+(\infty)$.

Lemma 2. *The number of edges is*

$$e = n_p + \deg_r^+ + \deg_c^+ + n_\infty + 2\varkappa\lfloor (m+1)/n \rfloor. \tag{11}$$

Lemma 3. *The number of faces is*

$$f = 2(n_\infty + n_c + \varkappa\lfloor (m+1)/n \rfloor - n_{cr}^+). \tag{12}$$

This lemma is valid for $n_c = n_{cr}^+ = 0$. Each part of spectrum curve between two CPs b_1, $b_2 \in \mathbb{R}_q^h$ increases the number of faces by one. So, this formula is valid for the case $n_{cr}^+ = 0$. Each additional CP $b \in C_q^{h+}$ increases the number of faces by $2(\deg^+(b)-1)$ and number parts of Spectrum Curves between this CP and other CPs by $2\deg^+(b)$.

Numbers of spectrum vertices, edges and faces, expressed by the formulas above, inserted to the Euler's characteristic's formula of sphere $v - e + f = 2$ give new relation.

Theorem 1. *The Euler's characteristic's formula is equivalent to*

$$\sum_{b\in\mathcal{B}} \deg^+(b) = \deg_r^+ + \deg_c^+ = n_\infty + 2n_c + n_{cr} - 1. \tag{13}$$

This formula was derived in [1] when there are no CPs in $\mathbb{C}_q^{h\pm}$ ($\deg_c^+ = 0$), all CPs are of the first order ($\deg_r^+ = 2n_{cr}$) and $n_c = 0$ in the case a), c). Then it can be rewritten as

$$n_{cr} = 2n_c + n_\infty - 1 = 2n_c + n - m - \varkappa - 1.$$

Corollary 1. *The number of edges is*

$$e = 2n_\infty + n_p + n_{cr} + 2n_c + 2\varkappa\lfloor (m+1)/n \rfloor - 1. \tag{14}$$

Remark 1. In the case $m+1 < n$ the formulas (10), (12)–(14) are

$$v = m + n_{cr} + 2n_{cr}^+ - n_{ce} + \varkappa, \qquad e = 2n - m - 2 + n_{cr} + 2n_c - n_{ce} - \varkappa,$$
$$f = 2(n - m - \varkappa + n_c - n_{cr}^+), \qquad \deg_r^+ + \deg_c^+ = n - m + 2n_c + n_{cr} - \varkappa - 1,$$

where n_{ce} is defined by (8).

In the case $m+1=n$ we have $n_\infty = 1-\varkappa$ and $n_p = n-2+\delta$, where $\delta = 1$ for the case d) and for $n\in\mathbb{N}_o$ in the case b), else $\delta=0$. So, for $m+1=n$ the following formulas

$$v = n + n_{cr} + 2n_{cr}^{+} - 1 + \delta, \qquad e = n + n_{cr} + 2n_c - 1 + \delta,$$
$$f = 2(1 + n_c - n_{cr}^{+}), \qquad \deg_r^{+} + \deg_c^{+} = 2n_c + n_{cr} - \varkappa$$

are valid.

Remark 2. If $n_{cr}^{+} = 0$ ($\deg_c^{+} = 0$) then $\deg_r^{+} - n_{cr} = 2n_c + n - m - \varkappa - 1 > n_{cr}$ shows that there exist CPs in $\mathbb{R}_q^h$ of the second or the higher order.

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REZIUMĖ

Diskrečiojo Šturmo ir Liuvilio uždavinio su nelokaliosiomis kraštinėmis sąlygomis spektrinių kreivių ir grafų teorijos sąsajos

J. Vitkauskas, A. Štikonas

Šturmo ir Liuvilio uždavinys su nelokaliosiomis kraštinėmis sąlygomis iškyla daugelyje mokslo šakų, tokiose kaip chemija, fizika ar biologija. Diskretizavus šį uždavinį bei išnagrinėjus spektrines kreives, galima įžvelgti grafų teorijos motyvų. Šiame straipsnyje pristatomos sąsajos tarp diskrečiojo Šturmo ir Liuvilio uždavinio su nelokaliosiomis kraštinėmis sąlygomis (poliai, kritiniai taškai ir spektrinės kreivės) bei grafų charakteristikų (viršūnės, briaunos ir veidai).

Raktiniai žodžiai: Šturmo ir Liuvilio uždavinys; spektrinės kreivės; nelokaliosios kraštinės sąlygos; grafai