**MSC 65M70** **DOI: 10.14529/jcem210304**

# NUMERICAL METHODS FOR SOLVING SPECTRAL PROBLEMS ON QUANTUM GRAPHS

***S. I. Kadchenko***[1]***,*** sikadchenko@mail.ru,
***A. V. Stavtseva***[2]***,*** asilina74@mail.ru,
***L. S. Ryazanova***[1]***,*** ryazanova2006@rambler.ru
[1] Nosov Magnitogorsk State Technical University, Magnitogorsk, Russian Federation
[2] Ural – Omega, Magnitogorsk, Russian Federation

Currently, many authors have developed a number of methods allowing to construct algorithms for the numerical solution of inverse spectral problems. However, from a computational point of view, most of the methods are ineffective, and serious computational difficulties arise in their application. Therefore, the development of new methods for solving spectral problems based on new approaches is urgent. In this article, new algorithms are developed for solving direct and inverse spectral problems defined on quantum graphs. In the developed algorithms, a special role is played by systems of eigenvalues and eigenfunctions of the corresponding unperturbed spectral problem, in which the potentials on all edges of the graph are equal to zero. With a large number of edges in the graph, finding these spectral characteristics faces a large amount of computation. Therefore, in the environment of the Maple package, a registered software package was also written to find the spectral characteristics of unperturbed problems defined on geometric graphs of any configuration and with any finite number of nodes. In the article, the methods for calculating the eigenvalues of discrete problems and solving inverse problems for semi-bounded operators defined on geometric graphs are illustrated by the example of the anthracene molecule.

Earlier, on the basis of the numerical methods of regularized traces and the Galerkin method, linear formulas were obtained for calculating the approximate eigenvalues of discrete semi-bounded operators defined on finite intervals. These formulas can be used to find approximate eigenvalues of discrete operators with any ordinal number without using eigenvalues with lower ordinal numbers. This removes many computational difficulties. Using these linear formulas, algorithms are developed for solving direct and inverse problems defined on quantum graphs, which is presented in the article.

The constructed algorithm for solving inverse spectral problems defined on sequential geometric graphs with a finite number of links was tested on the anthracene molecule. The algorithm allows to recover the values of unknown functions included in the operators at the discretization nodes using the eigenvalues of the operators and the spectral characteristics of the corresponding self-adjoint operators. The results of numerous experiments show good accuracy and computational efficiency of the developed method.

*Keywords: eigenvalues and eigenfunctions; discrete and self-adjoint operators; inverse spectral problems; Galerkin method; incorrectly set problems; Fredholm integral equation of the first kind; geometric graph.*

## Introduction

In connection with the need to create new technologies in science and technology, there is a need to develop computationally efficient methods for solving spectral problems for discrete semi-bounded operators defined on sets of various structures. One of these directions is associated with the quasi-one-dimensional motion of $\pi$-electrons in aromatic compounds [3]. Considering the width of the tubes in which electrons move to be small,

we can assume that they move along a network of one-dimensional conductors. This assumption is justified by the passage to the limit performed in the work [4]. A practical use of this approach for modelling a graphene molecule using quantum graphs can be found in the articles [5–8]. Let us outline the main provisions of new computational methods for solving direct and inverse spectral problems generated by discrete semi-bounded operators defined in a separable Hilbert space, which make it possible to model systems in molecules using quantum graphs on the examples of aromatic compounds.

In the works [9–14], a numerical method for calculating the eigenvalues of the boundary value problem

$$Lu = \mu u, \quad Gu|_{\Gamma} = 0, \tag{1}$$

was developed. Here $L$ is a discrete differential semi-bounded operator defined in a separable Hilbert space $H$ with the domain $D_L \in H$; $\Gamma$ is the boundary of the domain $D_L$. To calculate the eigenvalues of boundary value problem (1), we consider the sequence $\{H_n\}_{n=1}^{\infty}$ of finite-dimensional spaces, which is complete in $H$. Suppose that an orthonormal basis $\{\varphi_k\}_{k=1}^{n}$ of the spaces $H_n \subseteq H$ satisfy the homogeneous boundary conditions of problem (1). Following Galerkin method, an approximate solution to boundary value problem (1) is sought in the form

$$u_n = \sum_{k=1}^{n} a_k(n)\varphi_k. \tag{2}$$

The constants $a_k(n)$ are found so that the expression obtained after substituting $u_n$ instead of $u$ in equation (1) is orthonormal to the system of functions $\{\varphi_k\}_{k=1}^{n}$. The following theorems are proved in [13].

**Theorem 1.** *The Galerkin method applied to the problem on finding the eigenvalues of spectral problem* (1) *constructed on the system of functions* $\{\varphi_k\}_{k=1}^{\infty}$ *converges.*

**Theorem 2.** *The approximate eigenvalues* $\widetilde{\mu}_n$ *of spectral problem* (1) *are found by the linear formulas*

$$\widetilde{\mu}_n(n) = (L\varphi_n, \varphi_n) + \widetilde{\delta}_n, \ n \in N, \tag{3}$$

*where* $\widetilde{\delta}_n = \sum\limits_{k=1}^{n-1}[\widetilde{\mu}_k(n-1) - \widetilde{\mu}_k(n)]$, $\widetilde{\mu}_k(n)$ *is the n-th Galerkin approximation to the corresponding eigenvalues* $\mu_k$ *of spectral problem* (1).

In the same work, using Theorems 1 and 2, it was shown that

$$\lim_{n\to\infty} \widetilde{\delta}_n = 0. \tag{4}$$

To use formulas (3) when calculating the eigenvalues of problem (1), it is necessary to construct a system of coordinate functions $\{\varphi_k\}_{k=1}^{\infty}$, which satisfies boundary conditions (1). For this, the operator $L$ is represented in the form $L = T + P$, where $T$ is a self-adjoint differential operator of the same order as the operator $L$ with the domain $D_L$. Having found the eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$ and the eigenfunctions $\{v_n\}_{n=1}^{\infty}$ of the spectral problem

$$Tv = \lambda v, \quad Gv\,|_{\Gamma} = 0, \tag{5}$$

formulas (3) are written as

$$\widetilde{\mu}_n(n) = \lambda_n + (Pv_n, v_n) + \widetilde{\delta}_n,\ n \in \mathbb{N}. \tag{6}$$

If the system of eigenfunctions $\{v_n\}_{n=1}^{\infty}$ of problem (5) is not orthogonal, the functions $v_n$ must be expanded in Fourier series in terms of the system of functions $\{\varphi_k\}_{k=1}^{\infty}$. This allows to use formulas (6). Due to correct and uncomplicated calculations, algorithms for calculating eigenvalues by formulas (6) are simple and computationally efficient. Using the example of spectral problems generated by Sturm-Liouville operators of an arbitrary even order, it is shown that linear formulas (3) differ from the known asymptotic formulas only by the order of errors [14]. Compared to the classical methods for calculating the eigenvalues of discrete semi-bounded operators, finding them using formulas (6) drastically reduces the amount of calculations. Formula (6) allows to calculate the eigenvalues of discrete semi-bounded operators with any ordinal numbers, regardless of whether the eigenvalues with lower numbers are known or not.

Let us consider methods for solving inverse spectral problems on the example of differential operators $L_m$ defined in $L^2[a,b]$ of the form

$$L_m(u) = T_m(u) + P_m(u),$$

where $T_m(u) \equiv (-1)^{m+1}u^{(m)}$, $P_m(u) \equiv \sum\limits_{i=0}^{m-1} p_i(s)u^{(i)}$, $s \in [a,b]$, $m \in N$. It is assumed that all functions $p_i(s)$, $i = \overline{0, m-1}$ or some of them are not specified in the operators $L_m$. In the articles [11–14], a numerical method for solving inverse spectral problems was developed. For the known eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$, eigenfunctions $\{\varphi_n\}_{n=1}^{\infty}$ of unperturbed problem (5) and approximate eigenvalues $\{\widetilde{\mu}_n\}_{n=1}^{\infty}$ of perturbed spectral problem (1), the method allows to restore the values of unknown functions at the discretization nodes included in the operators $L_m$. To recover the values of the unknown functions $p_i(s)$, the developed algorithms use the required number of eigenvalues $\widetilde{\mu}_n$ belonging to the segments $[c_m, d_m]$. In the article [13] it is shown that to restore the values of the unknown functions $p_i(s)$, any segments $[c_m, d_m]$ can be chosen and this practically does not affect the accuracy of restoring the values of the functions $p_i(s)$ at discretization nodes. Note also that the technique described below for solving inverse spectral problems is applicable, with the corresponding changes, to solve inverse spectral problems generated by partial differential operators.

Based on formulas (6) for the operators $L_m$, we construct the Fredholm integral equations of the first kind in the matrix form

$$A_m(P_m) \equiv \int\limits_a^b K_m(x,s)P_m(s)ds = \widetilde{f}(x),\ x \in [c,d]. \tag{7}$$

Here $K_m(x_k,s) = \left(\varphi_k^{(m-1)}(s)\varphi_k(s)\ \ \ldots\ \ \varphi_k'(s)\varphi_k(s)\ \ \varphi_k^2(s)\right)$ are row matrices, and $P_m(s) = (p_{m-1}(s)\ \ p_{m-2}(s)\ldots p_0(s))^T$ are column matrices. Moreover, $K_m(x,s)$, $P_m(s)$ and $\widetilde{f}(x)$ are such that

$$\begin{gathered} K_m(x_k,s)P_m(s) = \sum_{i=0}^{m-1} p_i(s)\varphi_k^{(i)}(s)\varphi_k(s),\ a \le s \le b, \\ \widetilde{f}(x_k) = \widetilde{\mu}_k - \lambda_k - \widetilde{\delta}_k,\ c \le x_k \le d. \end{gathered} \tag{8}$$

If for solutions $P_m$ to equations (7) the residuals $||A_m(P_m) - \widetilde{f}||_{L_2[c,d]} = 0$, then the solutions are called exact. However, such solutions may not exist or may not be unique. Therefore, the concept of pseudo-solution was introduced. Solutions $P_m$ to equations (7) are called pseudo-solutions if they minimize the residuals $||A_m(P_m) - \tilde{f}||_{L_2[c,d]}$. Further, by solutions to Fredholm integral equations of the first kind (7) we mean pseudo-solutions. The exact values of the right-hand sides of equations (7) are unknown, but approximate values of $\widetilde{f}(x)$ are such that $||f - \widetilde{f}||^2_{L_2[c,d]} \leq \delta$. Suppose that the kernels $K_m(x,s)$ of integral equations (7) are continuous and closed in $\Pi = [c,d] \times [a,b]$ and $P_m(s) \in W_2^m[a,b]$, $\widetilde{f}(x) \in L_2[c,d]$. The problems of solving Fredholm integral equations of the first kind (7) are ill-posed. In the general case, their approximate solutions can be found only numerically using regularization method of A.N. Tikhonov and finite-difference approximation method. Very often it is possible to obtain good approximate solutions to integral equations (7) when discretizing them by applying regularization methods directly to systems of linear equations.

To discretize the domain $\Pi$, two grids are introduced along the $s$ and $x$ axes, which are uniform along the $s$ axis and non-uniform along the $x$ axis

$$s_1 = a, \quad s_{n+1} = s_n + h_s, \quad n = \overline{1, N_s - 1}, \quad h_s = \frac{b-a}{N_s - 1},$$

$$c = x_1 < x_2 < \ldots < x_{N_x} = d, \quad h_{x_1} = h_{x_2},$$

$$h_{x_k} = x_k - x_{k-1}, \quad k = \overline{2, N_x}, \quad N_x = mN_s.$$

To uniquely find $mN_s$ approximate values of the functions $p_i(s)$, $i = \overline{0, m-1}$ at the discretization nodes $\{s_n\}_{n=1}^{N_s}$ of the interval $[a,b]$ using the linear algebraic equations obtained during discretization of integral equations (1), it is necessary to know $mN_s$ approximate eigenvalues $\widetilde{\mu}_k$ of spectral problem (1) belonging to the segment $[c,d]$. We assume that they are known. At the same time, the following notation is introduced: $c = \widetilde{\mu}_{k_c}$, $d = \widetilde{\mu}_{k_d}$, $k_d = k_c + N_x - 1$.

To discretize equations (7), the functions $p_i(s)$ are interpolated by the Lagrange polynomials

$$p_i(s) = \sum_{n=1}^{N_s} l_n(s) p_{i_n}, \quad l_n(s) = \prod_{\substack{j=1 \\ j \neq n}}^{N_s} \frac{s - s_j}{s_n - s_j}, \; i = \overline{0, m-1}. \tag{9}$$

Substituting (9) into (7), we obtain systems of linear algebraic equations for the values of the functions $p_i(s)$ at the discretization nodes $p_{i_n} = p_i(s_n)$

$$\sum_{n=1}^{N_s} \sum_{i=0}^{m-1} H_{kn}^{(i)} p_{i_n} = \widetilde{\mu}_k, \; k = \overline{k_c, k_d}, \tag{10}$$

where $H_{kn}^{(i)} = \int\limits_a^b l_n(s) \varphi_k^{(i)}(s) \varphi_k(s) ds$, $i = \overline{0, m-1}$.

Let us write systems of linear equations (10) in the matrix form

$$A_{N_x} P_{N_x} = \widetilde{F}_{N_x}. \tag{11}$$

Here $A_{N_x}$ is a square matrix of the order $N_x \times N_x$, and $P_{N_x}$ and $\widetilde{F}_{N_x}$ are column matrices.

$$A_{N_x} = \begin{pmatrix} H_{11}^{(0)} & \dots & H_{1N_s}^{(0)} & H_{11}^{(1)} & \dots & H_{1N_s}^{(1)} & \dots & H_{11}^{(m-1)} & \dots & H_{1N_s}^{(m-1)} \\ H_{21}^{(0)} & \dots & H_{2N_s}^{(0)} & H_{21}^{(1)} & \dots & H_{2N_s}^{(1)} & \dots & H_{21}^{(m-1)} & \dots & H_{2N_s}^{(m-1)} \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ H_{N_s1}^{(0)} & \dots & H_{N_sN_s}^{(0)} & H_{N_s1}^{(1)} & \dots & H_{N_sN_s}^{(1)} & \dots & H_{N_s1}^{(m-1)} & \dots & H_{N_sN_s}^{(m-1)} \end{pmatrix},$$

$$P_{N_x} = \begin{pmatrix} p_{0_1} \\ \dots \\ p_{0_{N_s}} \\ \dots \\ p_{m_1} \\ \dots \\ p_{m_{N_s}} \end{pmatrix}, \quad \widetilde{F}_{N_x} = \begin{pmatrix} \widetilde{\mu}_{k_c} \\ \widetilde{\mu}_{k_c+1} \\ \dots \\ \widetilde{\mu}_{k_d} \end{pmatrix}.$$

In cases when some functions $p_i(s)$ in the operators $P_m(u)$ are given, then this should be taken into account when constructing systems of equations (11). It is clear that there is no need to search for the values of these functions at the discretization nodes of the segment $[a, b]$, and therefore the corresponding blocks are not included in the matrices $A_{N_x}$ and $P_{N_x}$, and the values of definite integrals, which integrands include these functions, pass with the opposite sign to the matrices $\widetilde{F}_{N_x}$. As a rule, the condition number $cond(A_{N_x})$ of matrices $A_{N_x}$ of systems of equations (11)) is relatively large, so we have ill-posed problems. Small errors in specifying the matrices $A_{N_x}$ and vectors $\widetilde{F}_{N_x}$ can lead to rather large errors in the vector of solutions $P_{N_x}$. In this regard, in order to partially eliminate the undesirable effects of errors, it is necessary to apply various regularization methods that allow replacing invalid solution vectors with some vectors of "of pseudo-solutions ", which are best for the problems under consideration.

Finding stable solutions close to normal pseudo-solutions to systems of linear algebraic equations (11) is based on the regularization method of A.N. Tikhonov with the choice of the regularization parameter by a residual. In our case, the regularization method of A.N. Tikhonov is reduced to minimizing parametric functionals of the form

$$||A_{N_x}P_{N_x} - \widetilde{F}_{N_x}||^2 + \alpha||P_{N_x}||^2, \tag{12}$$

where $\alpha > 0$ is a regularization parameter. The problem of minimizing (12) by $P_{N_x}$ is equivalent to solving systems of linear algebraic equations

$$(A_{N_x}^T A_{N_x} + \alpha I)\widetilde{P}_{N_x}^{\alpha} = A_{N_x}^T \widetilde{F}_{N_x}, \tag{13}$$

where the parameter $\alpha$ is chosen under the condition

$$||A_{N_x}\widetilde{P}_{N_x}^{\alpha} - \widetilde{F}_{N_x}|| = E||\widetilde{F}_{N_x}||. \tag{14}$$

The superscript $T$ means transposition, $E$ stands for the specified residual level, $||\widetilde{F}_{N_x}||$ is the Euclidean norm of the right-hand sides of equations (11), $I$ is the identity matrix.

The unique solution $\widetilde{P}_{N_x}^{\alpha}$ to the problem of minimizing functional (12) for a fixed $\alpha$ is expressed explicitly by the formula [15]:

$$\widetilde{P}_{N_x}^{\alpha} = \left(A_{N_x}^T A_{N_x} + \alpha I\right)^{-1} A_{N_x}^T F_{N_x}. \tag{15}$$

For $\alpha \to 0$, the solution $\widetilde{P}^{\alpha}_{N_x}$ converges to the normal solution to system (11) [15]. In (15), the inverse matrix exists for any rank of the matrix $A_{N_x}$ and any $\alpha > 0$.

Expression (15) for calculating $\widetilde{P}^{\alpha}_{N_x}$ can be represented in another form using the Sherman – Morrison – Woodbury formula [16]

$$\widetilde{P}^{\alpha}_{N_x} = \frac{1}{\alpha}\Big(I - A^T_{N_x}(\alpha I + A_{N_x}A^T_{N_x})\Big)^{-1} A^T_{N_x}\widetilde{F}_{N_x}. \tag{16}$$

In the case when the approximate solutions to integral equations (7) found by formulas (15) and (16) give a large residual, it is necessary to use the regularization method, which recommends to use the matrix functions $\widetilde{P}^{\alpha}_{m}$ as approximate solutions realizing the minimum values of smoothing functionals

$$\Phi_m[P_m, \widetilde{f}] = \int\limits_c^d \Big(A_m(P_m) - \widetilde{f}\Big)^2 dx + \alpha\Omega_m[P_m], \tag{17}$$

where $\alpha > 0$ is the regularization parameter, $\Omega_m[\widehat{P}_m] = \int\limits_a^b (P^T_m P_m + qP'^T_m P'_m)ds$ is the stabilizing Tikhonov functional, the value $q \geq 0$ determines the order of regularization, the superscript $T$ means that the matrix is transposed. For $q = 0$, instead of an incorrect equation of the first kind, an equation of the second kind is solved, while an integro-differential equation is solved for $q \neq 0$.

An approximate solution $P^{\alpha}_m$ is sought from the condition that the functional (17) reaches its minimum value, that is,

$$\Phi_m[P^{\alpha}_m, \widetilde{f}] = \inf_{P^{\alpha}_m \in W^m_2[a,b]} \Phi_m[P^{\alpha}_m, \widetilde{f}]. \tag{18}$$

under homogeneous boundary conditions

$$P'^{\alpha}_m(a) = \widehat{0}, \quad P'^{\alpha}_m(b) = \widehat{0}. \tag{19}$$

In this case, the equations defining the extremals of the functionals $\Phi_m[P^{\alpha}_m, \widetilde{f}]$ have the form:

$$\alpha[(P^{\alpha}_m)^T(t) - q\alpha[(P^{\alpha\prime\prime}_m)^T(t)] + \int\limits_a^b (P^{\alpha}_m)^T(s)R_m(t,s)ds = \widetilde{F}_m(t), \quad a \leq t \leq b. \tag{20}$$

Here $R_m(s,t) = \int\limits_c^d K^T_m(x,s)K_m(x,t)dx$, $\widetilde{F}_m(t) = \int\limits_c^d K_m(x,t)\widetilde{f}(x)dx$. The generalized residual method is used to select the regularization parameter $\alpha$.

Approximate numerical solutions $P^{\alpha}_m$ are found by the quadrature method, passing to finite spaces. For this, discretization grids along the $s$ and $x$ axes introduced earlier are

used. Denote $P^{\alpha}_{m_n} = P^{\alpha}_m(s_n)$, $K^{kn}_m = K(x_k, s_n)$, $\widetilde{f}_k = \widetilde{f}x_k$. Then

$$\int\limits_a^b (P^{\alpha}_m)^T(s) R_m(t,s)ds = \int\limits_a^b (P^{\alpha}_m)^T(s))\Big[\int\limits_c^d K^T_m(x,s)K_m(x,t)dx\Big]ds =$$

$$= \int\limits_a^b \sum_{n=1}^{N_s} l_n(s)\Big(p_{m-1_n})^{\alpha}(s) \;\; p^{\alpha}_{m-2_n}(s) \;\; \dots \;\; p^{\alpha}_{0_n}(s)\Big) \sum_{k=1}^{N_x} \gamma_k \times$$

$$\times \begin{pmatrix} K_{m-1}(x_k,t)K_{m-1}(x_k,s) & K_{m-1}(x_k,t)K_{m-2}(x_k,s)\dots K_{m-1}(x_k,t)K_0(x_k,s) \\ K_{m-2}(x_k,t)K_{m-1}(x_k,s) & K_{m-2}(x_k,t)K_{m-2}(x_k,s)\dots K_{m-2}(x_k,t)K_0(x_k,s) \\ \dots \;\; \dots \;\; \dots \;\; \dots & \dots \;\; \dots \;\; \dots \;\; \dots \;\; \dots \\ K_0(x_k,t)K_{m-1}(x_k,s) & K_0(x_k,t)K_{m-2}(x_k,s)\dots K_0(x_k,t)K_0(x_k,s) \end{pmatrix} ds =$$

$$= \sum_{n=1}^{N_s}\sum_{k=1}^{N_x}\gamma_k \sum_{i=1}^{m-1} H^{(i)}_{kn} p^{\alpha}_{i_n}\Big(K_{m-1}(x_k,t) \;\; K_{m-2}(x_k,t)\dots K_0(x_k,t)\Big), \tag{21}$$

where $\gamma_k$ are weight factors in quadrature formulas of trapezoids with variable step $h_{x_k}$. Therefore,

$$\int\limits_a^b (P^{\alpha}_m)^T(s) R_m(t,s)ds = \sum_{n=1}^{N_s}\sum_{i=1}^{m-1} G^{(li)}_n(t) p^{\alpha}_{i_n}, \;\; l = \overline{1, m-1}. \tag{22}$$

Here $G^{(li)}_n(t) = \sum\limits_{k=1}^{N_x} \gamma_k K_l(x_k,t) H^{(i)}_{kn}$.

Further

$$\alpha[(P^{\alpha}_m)^T(t) - q\alpha[(P^{\alpha\prime\prime}_m)^T(t)] = \alpha\sum_{n=1}^{N_s}[l_n(t) - ql^{''}_l(t)]\Big(p_{m-1_n})^{\alpha}(s) \;\; p^{\alpha}_{m-2_n}(s)\dots p^{\alpha}_{0_n}(s)\Big). \tag{23}$$

$$\widetilde{F}_m = \int\limits_c^d K_m(x,t)\widetilde{f}(x)dx = \Big(\widetilde{F}_{m-1}(t) \;\; \widetilde{F}_{m-2}(t)\dots\widetilde{F}_0(t)\Big). \tag{24}$$

Here $\widetilde{F}_i(t) = \sum\limits_{k=1}^{N_x} \gamma_k K_i(x_k,t)\widetilde{f}_k$, $i = \overline{0, m-1}$.

Using the obtained approximations (22) – (23), we write an approximate analogue of Tikhonov equations (20) in scalar form

$$\begin{cases} \sum\limits_{n=1}^{N_s}\Big\{\alpha\Big[l_n(t) - ql''_n(t)\Big]p^{\alpha}_{m-1_n} + \sum\limits_{i=0}^{m-1} G^{i,m-1}_n(t)p^{\alpha}_{i_n}\Big\} = \widetilde{F}_{m-1}(t) \\ \sum\limits_{n=1}^{N_s}\Big\{\alpha\Big[l_n(t) - ql''_n(t)\Big]p^{\alpha}_{m-2_n} + \sum\limits_{i=0}^{m-1} G^{i,m-2}_n(t)p^{\alpha}_{i_n}\Big\} = \widetilde{F}_{m-2}(t) \\ \dots \;\; \dots \;\; \dots \;\; \dots \;\; \dots \;\; \dots \;\; \dots \;\; \dots \;\; \dots \\ \sum\limits_{n=1}^{N_s}\Big\{\alpha\Big[l_n(t) - ql''_n(t)\Big]p^{\alpha}_{0_n} + \sum\limits_{i=0}^{m-1} G^{i0}_n(t)p^{\alpha}_{i_n}\Big\} = \widetilde{F}_0(t). \end{cases} \tag{25}$$

On the basis of the described technique for solving inverse spectral problems defined on finite intervals, we construct algorithms for solving direct and inverse spectral problems defined on quantum graphs.

## 1. Direct Spectral Problems in Quantum Graph Models

Based on formulas (6), we construct algorithms for calculating the eigenvalues of discrete semi-bounded operators defined on geometric graphs [14]. Consider a finite directed connected graph $\mathbf{G} = \mathbf{G}(\mathbf{V}, \mathbf{E})$ with connected edges. Let $\mathbf{V} = \{V_i\}_{i=1}^{i_0}$ be the set of vertices of the graph $\mathbf{G}$, and $\mathbf{E} = \{E_j\}_{j=1}^{j_0}$ be the set of its edges. Moreover, each edge $E_j$ has length $l_j > 0$. Suppose that the following discrete semi-bounded vector operator is given on the edges $E_j$, $j = \overline{1, j_0}$, of the graph $\mathbf{G}$:

$$\mathbf{L} = \Big(L_1, L_2, ..., L_{j_0}\Big), \tag{26}$$

which acts in the Hilbert space

$$\mathbf{H} = L_2(\mathbf{G}) = \{\mathbf{G} = (G_1, G_2, ..., G_{j_0}),\ G_j \in L_2(0, l_j),\ j = \overline{1, j_0}\}$$

with the scalar product

$$(\mathbf{g}, \mathbf{f}) = \sum_{j=1}^{j_0} \int_0^{l_j} g_j f_j ds_j,\ \mathbf{g}, \mathbf{f} \in \mathbf{H}. \tag{27}$$

Here $L_j$ are operators specified in $L_2[0, l_j], j = \overline{1, j_0}$.

Further, we assume that the vector operator $\mathbf{L}$ has the form $\mathbf{L} = \mathbf{T} + \mathbf{P}$, where $\mathbf{T}\boldsymbol{\psi} = \Big(T_1\psi_1, T_2\psi_2, ..., T_{j_0}\psi_{j_0}\Big)$, $T_j\psi_j = -\dfrac{d^2\psi_j}{ds_j^2}$, $\boldsymbol{P}\boldsymbol{\psi} = \Big(p_1(s_1)\psi_1, p_2(s_2)\psi_2, ..., p_{j_0}(s_{j_0})\psi_{j_0}\Big)$, $s_j \in [0, l_j]$, $j = \overline{1, j_0}$, $\boldsymbol{\psi} = (\psi_1, ..., \psi_{j_0})$, $\psi_j \in W_2^2[0, l_j]$ are twice continuously differentiable functions on the corresponding edge $E_j$ of the graph $\mathbf{G}$. At each vertex $V_i$ of the graph $\mathbf{G}$ for the vector functions $\boldsymbol{\psi}$, we define the boundary conditions

$$\sum_{E_k \in E^\alpha(V_s)} \frac{d\psi_k}{ds_k}\Big|_{s_k=0} - \sum_{E_m \in E^\omega(V_s)} \frac{d\psi_m}{ds_m}\Big|_{s_m=l_m} = 0, \tag{28}$$

$$\psi_i(0) = \psi_k(0) = \psi_m(l_m) = \psi_h(l_h). \tag{29}$$

Here $E_i, E_k \in E^\alpha(V_s)$, $E_m, E_h \in E^\omega(V_s)$, $E^\alpha(V_s)$ is the set of arcs starting at the vertex $V_s$, $E^\omega(V_s)$ is the set of arcs ending at the vertex $V_s$. Conditions (28) mean that the flow through each vertex must be zero, and (29) means that the solution $\boldsymbol{\psi} = (\psi_1, \psi_2, ..., \psi_{j_0})$ at each vertex must be continuous.

To construct the orthonormal system $\{\boldsymbol{\varphi}_n = (\varphi_{1_n}, \varphi_{2_n}, ..., \varphi_{j_{0_n}})\}_{n=1}^{\infty}$ of vector functions that satisfies boundary conditions (28), (29), consider the following direct spectral problem for the operator $\mathbf{T}$ on the graph $\mathbf{G}$:

$$\mathbf{T}\boldsymbol{\varphi} = \lambda\boldsymbol{\varphi}. \tag{30}$$

$$\sum_{E_k \in E^\alpha(V_s)} \frac{d\varphi_k}{ds_k}\Big|_{s_j=0} - \sum_{E_m \in E^\omega(V_s)} \frac{d\varphi_m}{ds_m}\Big|_{s_m=l_m} = 0, \tag{31}$$

$$\varphi_i(0) = \varphi_k(0) = \varphi_m(l_m) = \varphi_h(l_h). \tag{32}$$

Let $\{\lambda_n\}_{n=1}^{\infty}$ be the eigenvalues of problem (30) – (32) numbered in non-decreasing order of their values, and $\{\boldsymbol{\varphi}_n = (\varphi_{1_n}, \varphi_{2_n}, ..., \varphi_{j_{0_n}})\}_{n=1}^{\infty}$ be eigenvectors corresponding

to these eigenvalues $\lambda_n$. Finding the eigenvalues $\lambda_n$ and the corresponding eigenvectors $\boldsymbol{\varphi}_n$ of spectral problems (30) – (32) for any finite closed graphs with a large number of vertices causes great difficulties. Therefore, in the environment of the Maple mathematical package, a software package was written that allows to find the required number of these spectral characteristics for any finite graphs [17]. For clarity, the method for calculating

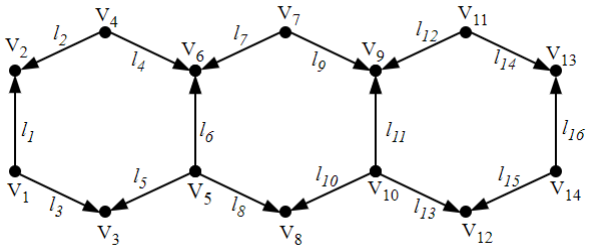


**Fig. 1**. Partitioning a directed graph for anthracene into vertices and edges

the eigenvalues of discrete semi-bounded operators given on geometric graphs is illustrated by the example of the anthracene molecule $C_{14}H_{10}$. The graph modelling the anthracene molecule consists of $i_0 = 14$ vertices and $j_0 = 16$ edges (see Fig. 1). Since the lengths of all edges for the anthracene molecule are the same, we can assume that $l_j = 1$ for all $j = \overline{1, j_0}$.

General solutions to differential equations

$$-\frac{d^2\varphi_j}{ds_j^2} = \lambda\varphi_j,\ j = \overline{1, j_0} \tag{33}$$

have the form

$$\varphi_j(s_j) = A_j \sin(\sqrt{\lambda}s_j) + B_j \cos(\sqrt{\lambda}s_j). \tag{34}$$

Using the written software package, a transcendental equation is obtained for finding the eigenvalues $\lambda_n$ of spectral problem (30) – (32) for the anthracene molecule

$$\begin{gathered} 62\sin(\sqrt{\lambda}) + 190\sin(3\sqrt{\lambda}) + 384\sin(5\sqrt{\lambda}) + 463\sin(7\sqrt{\lambda}) + \\ +415\sin(9\sqrt{\lambda}) + 225\sin(11\sqrt{\lambda}) + 81\sin(13\sqrt{\lambda}) = 0. \end{gathered} \tag{35}$$

Any eigenvalues $\lambda_n$ are roots of transcendental equation (35). The components $\varphi_{j_n}$ of the eigenvectors $\boldsymbol{\varphi}_n$ corresponding to the found eigenvalues $\lambda_n$ have the form

$$\varphi_{j_n} = C_n\Big(A_{j_n}\sin(\sqrt{\lambda_n}s_j) + B_{j_n}\cos(\sqrt{\lambda_n}s_j)\Big),\ j = \overline{1, 16}. \tag{36}$$

Here

$$A_{1_n} = \frac{4}{a_n}\Big(8\sin(\sqrt{\lambda_n}) + 23\sin(3\sqrt{\lambda_n}) + 16\sin(5\sqrt{\lambda_n}) + 9\sin(7\sqrt{\lambda_n})\Big),$$

$$B_{1_n} = \frac{4}{b_n}\Big(58 + 88\cos(2\sqrt{\lambda_n}) + 49\cos(4\sqrt{\lambda_n}) + 9\cos(6\sqrt{\lambda_n})\Big),$$

$$A_{2_n} = \frac{4}{a_n}\Big(26\sin(\sqrt{\lambda_n}) + 61\sin(3\sqrt{\lambda_n}) + 48\sin(5\sqrt{\lambda_n}) + 21\sin(7\sqrt{\lambda_n})\Big),$$

$$B_{2_n} = \frac{4}{b_n}\Big(16 + 30\cos(2\sqrt{\lambda_n}) + 15\cos(4\sqrt{\lambda_n}) + 7\cos(6\sqrt{\lambda_n})\Big),$$

$$A_{3_n} = -\frac{4}{a_n}\Big(8\sin(\sqrt{\lambda_n}) + 23\sin(3\sqrt{\lambda_n}) + 16\sin(5\sqrt{\lambda_n}) + 9\sin(7\sqrt{\lambda_n})\Big),$$

$$B_{3_n} = \frac{4}{b_n}\Big(58 + 88\cos(2\sqrt{\lambda_n}) + 49\cos(4\sqrt{\lambda_n}) + 9\cos(6\sqrt{\lambda_n})\Big),$$

$$A_{4n} = -\frac{4}{a_n}(26\sin(\sqrt{\lambda_n}) + 61\sin(3\sqrt{\lambda_n}) + 48\sin(5\sqrt{\lambda_n}) + 21\sin(7\sqrt{\lambda_n})),$$

$$B_{4_n} = \frac{12}{b_n}\Big(16 + 30\cos(2\sqrt{\lambda_n}) + 15\cos(4\sqrt{\lambda_n}) + 7\cos(6\sqrt{\lambda_n})\Big),$$

$$A_{5n} = \frac{4}{a_n}\Big(41\sin(\sqrt{\lambda_n}) + 85\sin(3\sqrt{\lambda_n}) + 80\sin(5\sqrt{\lambda_n}) + 37\sin(7\sqrt{\lambda_n}) + 9\sin(9\sqrt{\lambda_n}))\Big),$$

$$B_{5n} = \frac{4}{b_n}\Big(40 + 28\cos(6\sqrt{\lambda_n}) + 52\cos(4\sqrt{\lambda_n}) + 75\cos(2\sqrt{\lambda_n}) + 9\cos(8\sqrt{\lambda_n}))\Big),$$

$$A_{6n} = \frac{4}{a_n}\Big(5\sin(\sqrt{\lambda_n}) + 9\sin(3\sqrt{\lambda_n}) + 16\sin(5\sqrt{\lambda_n}) + 13\sin(7\sqrt{\lambda_n}) + 9\sin(9\sqrt{\lambda_n}))\Big),$$

$$B_{6n} = \frac{4}{b_n}\Big(40 + 28\cos(6\sqrt{\lambda_n}) + 52\cos(4\sqrt{\lambda_n}) + 75\cos(2\sqrt{\lambda_n}) + 9\cos(8\sqrt{\lambda_n}))\Big),$$

$$A_{7n} = \frac{2}{a_n}\Big(93\sin(\sqrt{\lambda_n}) + 212\sin(3\sqrt{\lambda_n}) + 214\sin(5\sqrt{\lambda_n}) + 124\sin(7\sqrt{\lambda_n}) + 45\sin(9\sqrt{\lambda_n})\Big),$$

$$B_{7n} = \frac{2}{b_n}\Big(64 + 99\cos(2\sqrt{\lambda_n}) + 127\cos(4\sqrt{\lambda_n}) + 73\cos(6\sqrt{\lambda_n}) + 45\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{8n} = -\frac{8}{a_n}\Big(23\sin(\sqrt{\lambda_n}) + 47\sin(3\sqrt{\lambda_n}) + 48\sin(5\sqrt{\lambda_n}) + 25\sin(7\sqrt{\lambda_n}) + 9\sin(9\sqrt{\lambda_n}))\Big),$$

$$B_{8n} = \frac{4}{b_n}\Big(40 + 28\cos(6\sqrt{\lambda_n}) + 52\cos(4\sqrt{\lambda_n}) + 75\cos(2\sqrt{\lambda_n}) + 9\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{9n} = -\frac{2}{a_n}\Big(93\sin(\sqrt{\lambda_n}) + 212\sin(3\sqrt{\lambda_n}) + 214\sin(5\sqrt{\lambda_n}) + 124\sin(7\sqrt{\lambda_n}) + 45\sin(9\sqrt{\lambda_n}))\Big),$$

$$B_{9n} = \frac{2}{b_n}\Big(64 + 99\cos(2\sqrt{\lambda_n}) + 127\cos(4\sqrt{\lambda_n}) + 73\cos(6\sqrt{\lambda_n}) + 45\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{10_n} = \frac{2}{a_n}\Big(217\sin(3\sqrt{\lambda_n}) + 76\sin(\sqrt{\lambda_n}) + 234\sin(5\sqrt{\lambda_n}) + 185\sin(7\sqrt{\lambda_n}) + 27\sin(11\sqrt{\lambda_n}) + 87\sin(9\sqrt{\lambda_n})\Big),$$

$$B_{10_n} = \frac{2}{b_n}\Big(29 + 84\cos(2\sqrt{\lambda_n}) + 101\cos(4\sqrt{\lambda_n}) + 107\cos(6\sqrt{\lambda_n}) + 27\cos(10\sqrt{\lambda_n}) + 60\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{11_n} = -\frac{2}{a_n}\Big( \sin(3\sqrt{\lambda_n}) + 8\sin(\sqrt{\lambda_n}) - 30\sin(5\sqrt{\lambda_n}) - 63\sin(7\sqrt{\lambda_n}) - $$

$$-27\sin(11\sqrt{\lambda_n}) - 51\sin(9\sqrt{\lambda_n})\Big),$$

$$B_{11_n} = \frac{2}{b_n}\Big(29 + 84\cos(2\sqrt{\lambda_n}) + 101\cos(4\sqrt{\lambda_n}) + 107\cos(6\sqrt{\lambda_n}) + 27\cos(10\sqrt{\lambda_n}) + $$

$$+60\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{12_n} = \frac{1}{a_n}\Big(291\sin(3\sqrt{\lambda_n}) + 103\sin(\sqrt{\lambda_n}) + 392\sin(5\sqrt{\lambda_n}) + 371\sin(7\sqrt{\lambda_n}) + $$

$$+81\sin(11\sqrt{\lambda_n}) + 216\sin(9\sqrt{\lambda_n})\Big),$$

$$B_{12_n} = \frac{3}{b_n}\Big(5+45\cos(2\sqrt{\lambda_n}))+60\cos(4\sqrt{\lambda_n})+84\cos(6\sqrt{\lambda_n})+27\cos(10\sqrt{\lambda_n})+51\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{13_n} = -\frac{4}{a_n}\Big(108\sin(3\sqrt{\lambda_n}) + 34\sin(\sqrt{\lambda_n}) + 132\sin(5\sqrt{\lambda_n}) + 124\sin(7\sqrt{\lambda_n}) + $$

$$+27\sin(11\sqrt{\lambda_n}) + 69\sin(9\sqrt{\lambda_n})\Big),$$

$$B_{13_n} = \frac{2}{b_n}\Big(29 + 84\cos(2\sqrt{\lambda_n}) + 101\cos(4\sqrt{\lambda_n}) + 107\cos(6\sqrt{\lambda_n}) + $$

$$+27\cos(10\sqrt{\lambda_n}) + 60\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{14_n} = -\frac{1}{a_n}\Big(291\sin(3\sqrt{\lambda_n}) + 103\sin(\sqrt{\lambda_n}) + 392\sin(5\sqrt{\lambda_n}) + 371\sin(7\sqrt{\lambda_n}) + $$

$$+81\sin(11\sqrt{\lambda_n}) + 216\sin(9\sqrt{\lambda_n})\Big),$$

$$B_{14_n} = \frac{3}{b_n}\Big(5 + 45\cos(2\sqrt{\lambda_n}) + 60\cos(4\sqrt{\lambda_n}) + 84\cos(6\sqrt{\lambda_n}) + $$

$$+27\cos(10\sqrt{\lambda_n}) + 51\cos(8\sqrt{\lambda_n})\Big),$$

$$A_{15_n} = \frac{1}{a_n}\Big(266\sin(3\sqrt{\lambda_n})+105\sin(\sqrt{\lambda_n})+482\sin(5\sqrt{\lambda_n})+523\sin(7\sqrt{\lambda_n})+81\sin(13\sqrt{\lambda_n}) + $$

$$+225\sin(11\sqrt{\lambda_n}) + 442\sin(9\sqrt{\lambda_n})\Big), \quad B_{15_n} = 1,$$

$$A_{16_n} = \frac{1}{a_n}\Big(114\sin(3\sqrt{\lambda_n})+19\sin(\sqrt{\lambda_n})+286\sin(5\sqrt{\lambda_n})+403\sin(7\sqrt{\lambda_n})+81\sin(13\sqrt{\lambda_n}) + $$

$$+225\sin(11\sqrt{\lambda_n}) + 388\sin(9\sqrt{\lambda_n})\Big), \quad B_{16_n} = 1,$$

$$a_n = 43\cos(\sqrt{\lambda_n}) + 154\cos(3\sqrt{\lambda_n}) + 320\cos(5\sqrt{\lambda_n}) + 421\cos(7\sqrt{\lambda_n}) + $$

$$+225\cos(11\sqrt{\lambda_n}) + 81\cos(13\sqrt{\lambda_n}) + 388\cos(9\sqrt{\lambda_n}),$$

$$b_n = 16 + 11\cos(2\sqrt{\lambda_n}) + 143\cos(4\sqrt{\lambda_n}) + 177\cos(6\sqrt{\lambda_n}) + $$

$$+81\cos(12\sqrt{\lambda_n}) + 144\cos(10\sqrt{\lambda_n}) + 244\cos(8\sqrt{\lambda_n}).$$

The system $\{\boldsymbol{\varphi}_n\}_{n=1}^{\infty}$ of eigenvectors of spectral problem (30) – (32) is orthogonal on the graph $\boldsymbol{G}$. The factors $C_n$ are found from the condition of its normalization. Using formulas (3) and (27), it is easy to show that the approximate eigenvalues of the vector operator $\mathbf{L}$ acting in the separable Hilbert space $W_2^2(\mathbf{G})$ are found by the following formulas [14]:

$$\widetilde{\mu}_n(n) = \lambda_n + \sum_{j=1}^{j_0} \int_0^{l_j} p_j(s_j)\varphi_{j_n}^2(s_j)ds_j + \widetilde{\delta}_n,\ n \in N. \tag{37}$$

Here $\widetilde{\delta}_n(n) = \sum\limits_{k=1}^{n-1}[\widehat{\mu}_k(n-1) - \widehat{\mu}_k(n)]$, $\widehat{\mu}_k(n)$ are the $n$-th Galerkin approximations of the $k$-th eigenvalue. Further, on the basis of formulas (37) obtained, we construct a technique for solving inverse spectral problems defined on quantum graphs.

## 2. Inverse Spectral Problems in Quantum Graph Models

One of the important problems of nanotechnology is the creation of systems with desired properties. To solve them, it is necessary to develop algorithms for solving inverse spectral problems in models of quantum graphs. For clarity, we illustrate the algorithm using the example of the anthracene molecule $C_{14}H_{10}$ for which $i_0 = 14$, $j_0 = 16$ and $l_j = 1$, $d_j = 1$ for all $j = \overline{1, j_0}$.

Consider inverse spectral problem for the operator $\boldsymbol{L}$ (28) given on the connected graph $\mathbf{G} = \mathbf{G}(\mathbf{V}^e, \mathbf{E})$

$$-\frac{d^2\psi_j}{ds_j^2} + p_j(s_j)\psi_j = \mu\psi_j,\ s_j \in [0, l_j],\ j = \overline{1, j_0}, \tag{38}$$

$$\sum_{E_j \in E^{\alpha}(V_i)} \frac{d\psi_j}{ds_j}\Big|_{s_j=0} - \sum_{E_m \in E^{\omega}(V_i)} \frac{d\psi_m}{ds_m}\Big|_{s_m=l_m} = 0, \tag{39}$$

$$\psi_i(0) = \psi_k(0) = \psi_m(l_m) = \psi_h(l_h). \tag{40}$$

We assume that the functions $p_j$ are not specified, but the eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$ and the corresponding eigenvectors $\{\boldsymbol{\varphi}_n\}_{n=1}^{\infty}$ of unperturbed problem (30) – (32) and the required number of approximate eigenvalues $\widetilde{\mu}_n$ of perturbed problem (38) – (40) belonging to the segment $[c, d]$ are known. Based on the listed known spectral data, it is necessary to construct an algorithm that allows recovering the approximate values of the functions $p_j$ at the discretization nodes. For this, using linear formulas (37), we compose the Fredholm integral equation of the first kind

$$\sum_{j=1}^{j_0} \int_0^{l_j} K^j(x, s_j)p_j(s_j)ds_j = \widetilde{f}(x),\ x \in [c, d], \tag{41}$$

where $K^j(x_n, s_j) = \varphi_{j_n}^2(s_j)$, $\widetilde{f}(x_n) = \widetilde{\mu}_n - \lambda_n - \widetilde{\delta}_n$. Suppose that $\varphi_{j_n}(s_j)$ are continuous and closed in $\Pi = [c, d] \times [0, l_1] \times \cdots \times [0, l_{j_0}]$, $p_j(s_j) \in W_2^2[0, l_j]$ and $\widetilde{f}(x) \in L_2[c, d]$.

We write integral equation (41) in matrix form

$$B(P) \equiv \int_0^{l_{max}} K(x, s)P(s)ds = \widetilde{f}(x), \quad x \in [c, d]. \tag{42}$$

Here $l_{max} = \max\limits_{1\le j\le j_0}\{l_j\}$, $K(x_n, s_j) = \left(\varphi^2_{1_n}(s_1), \varphi^2_{2_n}(s_2), \ldots, \varphi^2_{j_{0_n}}(s_{j_0})\right)$ are row matrices, and $P(s) = \begin{pmatrix} \chi_1(s)p_1(s_1) \\ \ldots\ldots\ldots \\ \chi_{j_0}(s)p_{j_0}(s_{j_0}) \end{pmatrix}$ are column matrices, and $\chi_j(s) = \begin{cases} 1, & s \in [0, l_j], \\ 0, & s \notin [0, l_j], \end{cases} \quad j = \overline{1, j_0}.$
For anthracene molecule, $l_{max} = 1$, $j_0 = 16$.

The problem of solving Fredholm integral equation of the first kind (42) is ill-posed. To construct its approximate solution $P^\alpha$, we use the Tikhonov regularization method. To do this, we use the smoothing functional

$$\Phi_\alpha[P, \widetilde{f}] = \int\limits_c^d \left(B(P) - \widetilde{f}\right)^2 dx + \alpha\Omega[P], \tag{43}$$

where $\alpha > 0$ is the regularization parameter, $\Omega[P] = \int\limits_0^1 \sum\limits_{j=1}^{j_0} (P^T P + qP'^T P')ds$ is the stabilizing Tikhonov functional, the value $q \ge 0$ determines the order of regularization, the superscript $T$ means that the matrix is transposed. For $q = 0$, instead of an incorrect equation of the first kind, an equation of the second kind is solved, while an integro-differential equation is solved for $q \ne 0$.

An approximate solution $P^\alpha$ is sought from the condition that functional (43) reaches its minimum value, that is,

$$\Phi_\alpha[P^\alpha, \widetilde{f}] = \inf_{P^\alpha \in W_2^2} \Phi_\alpha[P^\alpha, \widetilde{f}]. \tag{44}$$

under the homogeneous boundary conditions

$$(P^\alpha)'(0) = 0, \quad (P^\alpha)'(1) = 0. \tag{45}$$

In this case, the system of linear equations determining the extremals $P^\alpha(s)$ of the functional (43) has the form

$$\begin{cases} \alpha\chi_1(t)[p_1^\alpha(t) - q(p_1^\alpha)''(t)] + \sum\limits_{j=1}^{j_0} \int\limits_0^{l_j} \chi_j(s) R_{j1}(s,t) p_j^\alpha(s) ds = \widetilde{F}_1(t), \\ \alpha\chi_2(t)[p_2^\alpha(t) - q(p_2^\alpha)''(t)] + \sum\limits_{j=1}^{j_0} \int\limits_0^{l_j} \chi_j(s) R_{j2}(s,t) p_j^\alpha(s) ds = \widetilde{F}_2(t), \\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots\ \ldots \\ \alpha\chi_{j_0}(t)[p_{j_0}^\alpha(t) - q(p_{j_0}^\alpha)''(t)] + \sum\limits_{j=1}^{j_0} \int\limits_0^{l_j} \chi_j(s) R_{jj_0}(s,t) p_j^\alpha(s) ds = \widetilde{F}_{j_0}(t), \end{cases} \tag{46}$$

Here

$$\int\limits_0^{l_j} R_{ji}(s,t) p_j^\alpha(s) ds = \int\limits_0^{l_j} p_j^\alpha(s) \Big[ \int\limits_c^d K^j(x,s) K^i(x,t) dx \Big] ds,$$

$$\widetilde{F}_j(t) = \int\limits_c^d K^j(x,t) \tilde{f}(x) dx, \ j, i = \overline{1, j_0}, \ t \in [0, l_j].$$

To find approximate values $p_j^\alpha(s_j)$ of unknown functions $p_j(s_j)$ at the discretization nodes $\{s_{j_n}\}_{n=1}^{N_s}$ solving system of linear equations (46), the quadrature method is used.

## 3. Computational Experiment

For an approximate numerical solution $p_j^\alpha$, it is necessary to pass to finite subspaces. We introduce discretization grids along the axes $s_j$ and $x$, which are uniform along the axis $s_j$ and non-uniform along the axis $x$

$$s_{j_1} = 0, \quad s_{j_{n+1}} = s_{j_n} + h_{s_j}, \quad n = \overline{1, N_{s_j} - 1}, \quad h_s = \frac{l_j}{N_{s_j} - 1},$$
$$c = x_1 < x_2 < \ldots < x_{N_x} = d, \quad h_1 = h_2,$$
$$h_k = x_k - x_{k-1}, \quad k = \overline{2, N_x - 1}.\ N_x = \sum_{j=1}^{j_0} N_{s_j}.$$

Let us use the described algorithm to find a solution to inverse spectral problem (38)–(40) given on a graph and simulating an anthracene molecule. For this purpose, a software package was written in the Maple mathematical environment that allows computational experiments to recover the operator $\boldsymbol{L}$ in the case when the functions $p_j(s_j)$ included in this operator are unknown.

Suppose that the eigenvalues $\{\lambda_n\}_{n=1}^\infty$ and the corresponding eigenvectors $\{\boldsymbol{\varphi}_n\}_{n=1}^\infty$ of unperturbed problem (30)–(32) and the required number $N_x$ of approximate eigenvalues $\widetilde{\mu}_n$ of perturbed problem (38)–(40) belonging to the segment $[c, d]$ are known.

In the previous section, it was shown that the eigenvalues $\{\lambda_n\}_{n=1}^\infty$ of spectral problem (30)–(32) for an anthracene molecule are the roots of transcendental equation (35), and the components of the eigenvectors $\{\boldsymbol{\varphi}_n\}_{n=1}^\infty$ are found by formulas (36).

Tables 1–8 show the results of recovering the values of the potentials $p_1(s_1) = \sin(2s_1 + I)$, $p_2(s_2) = \cos(s_2) + 2s_2 + e^{Is_2}$, $p_3(s_3) = e^{Is_3} + 1$, $p_4(s_4) = 5s_4 + I$, $p_5(s_5) = 5s_5 - I$, $p_6(s_6) = 0$, $p_7(s_7) = 5s_7 + I$, $p_8(s_8) = 5s_8 - I$, $p_9(s_9) = s_9^2 + 5I + 1$, $p_{10}(s_{10}) = s_{10}^2 + 5I - 1$, $p_{11}(s_{11}) = s_{11}^2 + 5s_{11}$, $p_{12}(s_{12}) = \cos(s) + 2s + e^{Is}$, $p_{13}(s_{13}) = e^{Is} + 1$ $p_{14}(s_{14}) = 5s_{14} + I$, $p_{15}(s_{15}) = 5s_{15} - I$, $p_{16}(s_{16}) = 0$, $l_j = 1$, $s_j \in [0, 1]$, $j = \overline{1, 16}$ given on the corresponding edges of the graph $\boldsymbol{G}$ using the developed algorithm. Here $I$ is imaginary unit.

**Table 1**

| $n$ | $p_1(s_{1_n})$ | $p_1^\alpha(s_{1_n})$ | $\zeta_{1_n}$ | $p_2(s_{2_n})$ | $p_2^\alpha(s_{2_n})$ | $\zeta_{2_n}$ |
|---|---|---|---|---|---|---|
| 1 | $0.000 + 1.175I$ | $0.000 + 1.175I$ | $1.814 \cdot 10^{-6}$ | $2.000 + 0.000I$ | $2.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $0.307 + 1.152I$ | $0.147 + 1.031I$ | $5.425 \cdot 10^{-5}$ | $2.190 + 0.100I$ | $2.123 + 0.081I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $0.601 + 1.082I$ | $0.461 + 1.004I$ | $1.655 \cdot 10^{-5}$ | $2.360 + 0.199I$ | $2.329 + 0.183I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $0.871 + 0.970I$ | $0.764 + 0.930I$ | $5.482 \cdot 10^{-5}$ | $2.511 + 0.296I$ | $2.492 + 0.282I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $1.107 + 0.819I$ | $1.042 + 0.815I$ | $8.821 \cdot 10^{-6}$ | $2.642 + 0.389I$ | $2.639 + 0.378I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $1.298 + 0.635I$ | $1.275 + 0.664I$ | $5.007 \cdot 10^{-5}$ | $2.755 + 0.479I$ | $2.772 + 0.472I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $1.438 + 0.426I$ | $1.469 + 0.480I$ | $3.872 \cdot 10^{-5}$ | $2.851 + 0.565I$ | $2.877 + 0.562I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $1.521 + 0.200I$ | $1.602 + 0.273I$ | $2.007 \cdot 10^{-5}$ | $2.930 + 0.644I$ | $2.973 + 0.647I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $1.542 - 0.034I$ | $1.676 + 0.052I$ | $8.243 \cdot 10^{-5}$ | $2.993 + 0.717I$ | $3.053 + 0.726I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $1.503 - 0.267I$ | $1.689 - 0.179I$ | $1.806 \cdot 10^{-5}$ | $3.043 + 0.783I$ | $3.110 + 0.798I$ | $1.806 \cdot 10^{-5}$ |

**Table 2**

| $n$ | $p_3(s_{3_n})$ | $p_3^\alpha(s_{3_n})$ | $\zeta_{3_n}$ | $p_4(s_{4_n})$ | $p_4^\alpha(s_{4_n})$ | $\zeta_{4_n}$ |
|---|---|---|---|---|---|---|
| 1 | $2.000 + 0.000I$ | $2.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ | $0.000 + 1.000I$ | $0.000 + 1.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $1.995 + 0.100I$ | $1.975 + 0.080I$ | $5.425 \cdot 10^{-5}$ | $0.500 + 1.000I$ | $0.471 + 1.004I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.980 + 0.199I$ | $1.975 + 0.182I$ | $1.655 \cdot 10^{-5}$ | $1.000 + 1.000I$ | $0.988 + 1.005I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.955 + 0.296I$ | $1.963 + 0.281I$ | $5.482 \cdot 10^{-5}$ | $1.500 + 1.000I$ | $1.481 + 1.002I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $1.921 + 0.389I$ | $1.931 + 0.377I$ | $8.821 \cdot 10^{-5}$ | $2.000 + 1.000I$ | $1.977 + 0.998I$ | $8.821 \cdot 10^{-5}$ |
| 6 | $1.878 + 0.479I$ | $1.914 + 0.473I$ | $5.007 \cdot 10^{-5}$ | $2.500 + 1.000I$ | $2.482 + 1.000I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $1.825 + 0.565I$ | $1.860 + 0.561I$ | $3.872 \cdot 10^{-5}$ | $3.000 + 1.000I$ | $2.972 + 0.998I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $1.765 + 0.644I$ | $1.817 + 0.648I$ | $2.007 \cdot 10^{-5}$ | $3.500 + 1.000I$ | $3.473 + 1.001I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $1.697 + 0.717I$ | $1.761 + 0.727I$ | $8.243 \cdot 10^{-5}$ | $4.000 + 1.000I$ | $3.973 + 1.004I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $1.622 + 0.783I$ | $1.678 + 0.798I$ | $1.806 \cdot 10^{-5}$ | $4.500 + 1.000I$ | $4.465 + 1.004I$ | $1.806 \cdot 10^{-5}$ |

**Table 3**

| $n$ | $p_5(s_{5_n})$ | $p_5^\alpha(s_{5_n})$ | $\zeta_{5_n}$ | $p_6(s_{6_n})$ | $p_6^\alpha(s_{6_n})$ | $\zeta_{6_n}$ |
|---|---|---|---|---|---|---|
| 1 | $0.000 - 1.000I$ | $0.000 - 1.000I$ | $1.814 \cdot 10^{-6}$ | $0.000 + 0.000I$ | $0.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $0.500 - 1.000I$ | $0.465 - 0.996I$ | $5.425 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.001I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.000 - 1.000I$ | $0.972 - 0.996I$ | $1.655 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.500 - 1.000I$ | $1.476 - 0.998I$ | $5.482 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $2.000 - 1.000I$ | $1.968 - 1.002I$ | $8.821 \cdot 10^{-6}$ | $0.000 + 0.000I$ | $0.029 - 0.001I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $2.500 - 1.000I$ | $2.486 - 0.999I$ | $5.007 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 - 0.001I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $3.000 - 1.000I$ | $2.974 - 1.002I$ | $3.872 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 - 0.001I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $3.500 - 1.000I$ | $3.483 - 0.998I$ | $2.007 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $4.000 - 1.000I$ | $3.987 - 0.995I$ | $8.243 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $4.500 - 1.000I$ | $4.471 - 0.996I$ | $1.806 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.001I$ | $1.806 \cdot 10^{-5}$ |

**Table 4**

| $n$ | $p_7(s_{7_n})$ | $p_7^\alpha(s_{7_n})$ | $\zeta_{7_n}$ | $p_8(s_{6_n})$ | $p_8^\alpha(s_{8_n})$ | $\zeta_{8_n}$ |
|---|---|---|---|---|---|---|
| 1 | $0.000 + 1.000I$ | $0.000 + 1.000I$ | $1.814 \cdot 10^{-6}$ | $0.000 - 1.000I$ | $0.000 - 1.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $0.500 + 1.000I$ | $0.480 + 0.996I$ | $5.425 \cdot 10^{-5}$ | $0.500 - 1.000I$ | $0.479 - 1.003I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.000 + 1.000I$ | $0.980 + 1.000I$ | $1.655 \cdot 10^{-5}$ | $1.000 - 1.000I$ | $0.980 - 1.000I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.500 + 1.000I$ | $1.479 + 1.002I$ | $5.482 \cdot 10^{-5}$ | $1.500 - 1.000I$ | $1.480 - 0.998I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $2.000 + 1.000I$ | $1.979 + 1.003I$ | $8.821 \cdot 10^{-6}$ | $2.000 - 1.000I$ | $1.979 - 0.997I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $2.500 + 1.000I$ | $2.479 + 1.004I$ | $5.007 \cdot 10^{-5}$ | $2.500 - 1.000I$ | $2.479 - 0.996I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $3.000 + 1.000I$ | $2.979 + 1.003I$ | $3.872 \cdot 10^{-5}$ | $3.000 - 1.000I$ | $2.979 - 0.997I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $3.500 + 1.000I$ | $3.480 + 1.002I$ | $2.007 \cdot 10^{-5}$ | $3.500 - 1.000I$ | $3.479 - 0.998I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $4.000 + 1.000I$ | $3.980 + 1.000I$ | $8.243 \cdot 10^{-5}$ | $4.000 - 1.000I$ | $3.980 - 1.000I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $4.500 + 1.000I$ | $4.479 + 0.997I$ | $1.806 \cdot 10^{-5}$ | $4.500 - 1.000I$ | $4.480 - 1.004I$ | $1.806 \cdot 10^{-5}$ |

**Table 5**

| $n$ | $p_9(s_{9_n})$ | $p_9^{\alpha}(s_{9_n})$ | $\zeta_{9_n}$ | $p_{10}(s_{10_n})$ | $p_{10}^{\alpha}(s_{10_n})$ | $\zeta_{10_n}$ |
|---|---|---|---|---|---|---|
| 1 | $1.00 + 5.00I$ | $1.000 + 5.000I$ | $1.814 \cdot 10^{-6}$ | $-1.000 + 5.000I$ | $-1.000 + 5.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $1.01 + 5.00I$ | $1.111 + 4.996I$ | $5.425 \cdot 10^{-5}$ | $-0.990 + 4.000I$ | $-0.890 + 4.997I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.04 + 5.00I$ | $1.121 + 5.000I$ | $1.655 \cdot 10^{-5}$ | $-0.960 + 5.000I$ | $-0.879 + 5.000I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.09 + 5.00I$ | $1.150 + 5.002I$ | $5.482 \cdot 10^{-5}$ | $-0.910 + 5.000I$ | $-0.849 + 5.002I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $1.16 + 5.00I$ | $1.200 + 5.003I$ | $8.821 \cdot 10^{-6}$ | $-0.840 + 5.000I$ | $-0.800 + 5.003I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $1.25 + 5.00I$ | $1.270 + 5.004I$ | $5.007 \cdot 10^{-5}$ | $-0.750 + 5.000I$ | $-0.730 + 5.004I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $1.36 + 5.00I$ | $1.360 + 5.003I$ | $3.872 \cdot 10^{-5}$ | $-0.640 + 5.000I$ | $-0.640 + 5.003I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $1.49 + 5.00I$ | $1.471 + 5.002I$ | $2.007 \cdot 10^{-5}$ | $-0.510 + 5.000I$ | $-0.530 + 5.002I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $1.64 + 5.00I$ | $1.601 + 5.000I$ | $8.243 \cdot 10^{-5}$ | $-0.360 + 5.000I$ | $-0.399 + 5.000I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $1.81 + 5.00I$ | $1.750 + 4.997I$ | $1.806 \cdot 10^{-5}$ | $-0.190 + 5.000I$ | $-0.249 + 4.996I$ | $1.806 \cdot 10^{-5}$ |

**Table 6**

| $n$ | $p_{11}(s_{11_n})$ | $p_{11}^{\alpha}(s_{11_n})$ | $\zeta_{11_n}$ | $p_{12}(s_{12_n})$ | $p_{12}^{\alpha}(s_{12_n})$ | $\zeta_{12_n}$ |
|---|---|---|---|---|---|---|
| 1 | $0.000 + 0.000I$ | $0.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ | $2.000 + 0.000I$ | $2.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $0.510 + 0.000I$ | $0.560 + 0.001I$ | $5.425 \cdot 10^{-5}$ | $2.190 + 0.100I$ | $2.123 + 0.081I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.040 + 0.000I$ | $1.070 + 0.000I$ | $1.655 \cdot 10^{-5}$ | $2.360 + 0.199I$ | $2.329 + 0.183I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.590 + 0.000I$ | $1.600 + 0.000I$ | $5.482 \cdot 10^{-5}$ | $2.511 + 0.296I$ | $2.492 + 0.282I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $2.160 + 0.000I$ | $2.150 - 0.001I$ | $8.821 \cdot 10^{-6}$ | $2.642 + 0.389I$ | $2.639 + 0.378I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $2.750 + 0.000I$ | $2.720 - 0.001I$ | $5.007 \cdot 10^{-5}$ | $2.755 + 0.479I$ | $2.772 + 0.472I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $3.360 + 0.000I$ | $3.310 - 0.001I$ | $3.872 \cdot 10^{-5}$ | $2.851 + 0.565I$ | $2.877 + 0.562I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $3.990 + 0.000I$ | $3.920 + 0.000I$ | $2.007 \cdot 10^{-5}$ | $2.930 + 0.644I$ | $2.973 + 0.647I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $4.640 + 0.000I$ | $4.550 + 0.000I$ | $8.243 \cdot 10^{-5}$ | $2.993 + 0.717I$ | $3.053 + 0.726I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $5.310 + 0.000I$ | $5.200 + 0.001I$ | $1.806 \cdot 10^{-5}$ | $3.043 + 0.783I$ | $3.110 + 0.798I$ | $1.806 \cdot 10^{-5}$ |

**Table 7**

| $n$ | $p_{13}(s_{13_n})$ | $p_{13}^{\alpha}(s_{13_n})$ | $\zeta_{13_n}$ | $p_{14}(s_{14_n})$ | $p_{14}^{\alpha}(s_{14_n})$ | $\zeta_{14_n}$ |
|---|---|---|---|---|---|---|
| 1 | $2.000 + 0.000I$ | $2.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ | $0.000 + 1.000I$ | $0.000 + 1.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $1.995 + 0.100I$ | $1.975 + 0.075I$ | $5.425 \cdot 10^{-5}$ | $0.500 + 1.000I$ | $0.471 + 1.004I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.980 + 0.199I$ | $1.975 + 0.168I$ | $1.655 \cdot 10^{-5}$ | $1.000 + 1.000I$ | $0.988 + 1.005I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.955 + 0.296I$ | $1.963 + 0.252I$ | $5.482 \cdot 10^{-5}$ | $1.500 + 1.000I$ | $1.481 + 1.002I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $1.921 + 0.389I$ | $1.931 + 0.343I$ | $8.821 \cdot 10^{-6}$ | $2.000 + 1.000I$ | $1.977 + 0.998I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $1.878 + 0.479I$ | $1.914 + 0.426I$ | $5.007 \cdot 10^{-5}$ | $2.500 + 1.000I$ | $2.482 + 1.000I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $1.825 + 0.565I$ | $1.860 + 0.508I$ | $3.872 \cdot 10^{-5}$ | $3.000 + 1.000I$ | $2.972 + 0.998I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $1.765 + 0.644I$ | $1.817 + 0.593I$ | $2.007 \cdot 10^{-5}$ | $3.500 + 1.000I$ | $3.473 + 1.001I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $1.697 + 0.717I$ | $1.761 + 0.665I$ | $8.243 \cdot 10^{-5}$ | $4.000 + 1.000I$ | $3.973 + 1.004I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $1.622 + 0.783I$ | $1.678 + 0.743I$ | $1.806 \cdot 10^{-5}$ | $4.500 + 1.000I$ | $4.465 + 1.004I$ | $1.806 \cdot 10^{-5}$ |

**Table 8**

| $n$ | $p_{15}(s_{15_n})$ | $p_{15}^{\alpha}(s_{15_n})$ | $\zeta_{15_n}$ | $p_{16}(s_{16_n})$ | $p_{16}^{\alpha}(s_{16_n})$ | $\zeta_{16_n}$ |
|---|---|---|---|---|---|---|
| 1 | $0.000 - 1.000I$ | $0.000 - 1.000I$ | $1.814 \cdot 10^{-6}$ | $0.000 + 0.000I$ | $0.000 + 0.000I$ | $1.814 \cdot 10^{-6}$ |
| 2 | $0.500 - 1.000I$ | $0.465 - 0.996I$ | $5.425 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.001I$ | $5.425 \cdot 10^{-5}$ |
| 3 | $1.000 - 1.000I$ | $0.972 - 0.996I$ | $1.655 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $1.655 \cdot 10^{-5}$ |
| 4 | $1.500 - 1.000I$ | $1.476 - 0.998I$ | $5.482 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $5.482 \cdot 10^{-5}$ |
| 5 | $2.000 - 1.000I$ | $1.968 - 1.002I$ | $8.821 \cdot 10^{-6}$ | $0.000 + 0.000I$ | $0.029 - 0.001I$ | $8.821 \cdot 10^{-6}$ |
| 6 | $2.500 - 1.000I$ | $2.486 - 0.999I$ | $5.007 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 - 0.001I$ | $5.007 \cdot 10^{-5}$ |
| 7 | $3.000 - 1.000I$ | $2.974 - 1.002I$ | $3.872 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 - 0.001I$ | $3.872 \cdot 10^{-5}$ |
| 8 | $3.500 - 1.000I$ | $3.483 - 0.998I$ | $2.007 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $2.007 \cdot 10^{-5}$ |
| 9 | $4.000 - 1.000I$ | $3.987 - 0.995I$ | $8.243 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.000I$ | $8.243 \cdot 10^{-5}$ |
| 10 | $4.500 - 1.000I$ | $4.471 - 0.996I$ | $1.806 \cdot 10^{-5}$ | $0.000 + 0.000I$ | $0.029 + 0.001I$ | $1.806 \cdot 10^{-5}$ |

Values $\zeta_{j_n} = |\widetilde{F}_j(s_{j_n}) - \int\limits_0^1 \sum\limits_{j=1}^{16} \Phi(x_n, s) P^{\alpha}(s) ds|$ define the pointwise absolute error of the approximate solution $P^{\alpha}(s)$. The residual of the obtained solution is $\xi = ||\widetilde{F}_j(x) - B(P_j^{\alpha})||_{L_2[c,d]} = 9.539 \cdot 10^{-8}$. Results of calculations found by numerical solution of system of equations (46) are shown in Tables 1–8. The value of the regularization parameter $\alpha = 7.049 \cdot 10^{-5}$ is found by the generalized residual method.

## Conclusion

Conducted computational experiments to restore approximate values $p_j^{\alpha}$ of the functions $p_j$, $j = \overline{1, 16}$ on a sixteen-edges geometric graph at discretization nodes from the known eigenvalues $\{\lambda_n\}_{n=1}^{\infty}$, eigenvectors $\{\boldsymbol{\varphi}_n\}_{n=1}^{\infty}$ of unperturbed problem (38)–(40) and the known approximate values $\widetilde{\mu}_n \in [c, d]$ of spectral problem (38)–(40) showed high computational efficiency of the developed technique for solving inverse spectral problems for perturbed self-adjoint operators defined on geometric graphs. It should be noted that the method of recovering the vector operator $\mathbf{L}$ can be easily transferred to the case of graphs with any configuration and with any finite number of links.

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*Sergey I. Kadchenko, DSc(Math), Professor, Department of Applied Mathematics and Informatics, Nosov Magnitogorsk State Technical University (Magnitogorsk, Russian Federation), sikadchenko@mail.ru.*

*Anastasiya V. Stavtseva, CJSC «Ural – Omega»(Magnitogorsk, Russian Federation), asilina74@mail.ru.*

*Lyubov S. Ryazanova, PhD(Education), Associate Professor, Department of Applied Mathematics and Computer Science, Nosov Magnitogorsk State Technical University (Magnitogorsk, Russian Federation), ryazanova2006@rambler.ru.*

*Received* August 20, 2021.

УДК 519.624.3 DOI: 10.14529/jcem210304

# ЧИСЛЕННЫЕ МЕТОДЫ РЕШЕНИЯ СПЕКТРАЛЬНЫХ ЗАДАЧ НА КВАНТОВЫХ ГРАФАХ

*С. И. Кадченко, А. В. Ставцева, Л. С. Рязанова*

В настоящее время многие авторы разработали ряд методов позволяющие построения алгоритмов численного решения обратных спектральных задач. Однако большинство методов с вычислительной точки зрения являются малоэффективными, и при их применении возникают серьезные вычислительные трудности. Поэтому разработка новых методов решения спектральных задач, построенных на новых подходах, является актуальной. В данной статье разработаны новые алгоритмы решения прямых и обратных спектральных задач, заданных на квантовых графах. Особую роль в разработанных алгоритмах играют системы собственных значений и собственных функций соответствующей, невозмущенной спектральной задачи, в которой на всех ребрах графа потенциалы равны нулю. Нахождение этих спектральных характеристик, при большом количестве ребер у графа, сталкивается с большими объемами вычислений. Поэтому в среде пакета Maple был написан и зарегистрированный пакет программ, позволяющий находить спектральные характеристики невозмущенных задач, заданных на геометрических графах, любой конфигурации и с любым конечным числом узлов. В статье, методики вычисления собственных значений дискретных и решения обратных задач для полуограниченных операторов, заданных на геометрических графах, проиллюстрированы на примере молекулы антрацена.

Ранее, на основе численных методов регуляризованных следов и метода Галеркина, были получены линейные формулы вычисления приближенных собственных значений дискретных полуограниченных операторов, заданных на конечных интервалах. По этим формулам можно находить приближенные собственные значения дискретных операторов с любым порядковых номером, не используя собственные значения с меньшими порядковыми номерами. Это снимает многие вычислительные трудности. Используя данные линейные формулы, разработаны алгоритмы решения прямых и обратных задач заданных на квантовых графах, что представлено в статье.

Построенный алгоритм решения обратных спектральных задач, заданных на последовательных геометрических графах с конечным числом звеньев, был апробирован на молекуле антрацена. Он позволяет восстанавливать в узлах дискретизации значения неизвестных функций, входящих в операторы, используя собственные значения операторов и спектральные характеристики соответствующих самосопряженных операторов. Результаты многочисленных экспериментов показали хорошую точность и вычислительную эффективность разработанного метода.

*Ключевые слова: собственные значения и собственные функции; дискретные и самосопряженные операторы; обратные спектральные задачи; метод Галеркина; некорректно поставленные задачи; интегральное уравнение Фредгольма первого рода; геометрический граф.*

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*Кадченко Сергей Иванович, доктор физико-математических наук, профессор, кафедра прикладной математики и информатики, Магнитогорский государственный технический университет им. Г. И. Носова (г. Магнитогорск, Российская Федерация), sikadchenko@mail.ru.*

*Ставцева Анастасия Викторовна, Урал – Омега (г. Магнитогорск, Российская Федерация), asilina74@mail.ru.*

*Рязанова Любовь Сергеевна, кандидат педагогических наук, доцент, кафедра прикладной математики и информатики, Магнитогорский государственный технический университет им. Г. И. Носова (г. Магнитогорск, Российская Федерация), ryazanova2006@rambler.ru.*

*Поступила в редакцию* 20 августа 2021 г.