

# THE CALCULATION OF VALUES OF EIGENFUNCTIONS OF THE PERTURBED SELF-ADJOINT OPERATORS BY REGULARIZED TRACES METHOD

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The authors developed a numerical non-iterative method of finding of the value of eigenfunctions of perturbed self-adjoint operators, which was called the method of regularized traces. It allows to find the value of eigenfunctions of perturbed discrete operators, using the spectral characteristics of the unperturbed operator and the eigenvalues of the perturbed operator. In contrast to the known methods, in the method of regularized traces the value of eigenfunctions are found by the linear equations. It significantly increases the computational efficiency. The difficulty of the method is to find sums of functional series of "suspended" corrections of perturbation theory, which can be found only numerically. The formulas, which are convenient to find "suspended" corrections such that one can approximate the amount of these functional series by summing up of them, are presented in the paper. However, if a norm of the perturbing operator is large, then the summation of "suspended" corrections can be not effective. We obtain analytical formulas, which allow to find the values of sums of functional series of "suspended" corrections of perturbation theory in the discrete nodes without direct summation of its terms. Computational experiments are performed. These experiments allowed to find the values of the eigenfunctions of the perturbed one-dimensional Laplace operator. The experimental results showed the accuracy and computational efficiency of the developed method.

*Keywords:* method of regularized traces; perturbed operators; eigenvalues; eigenfunctions; multiple spectrum; "suspended" corrections of perturbation theory.

## Introduction

The problem of finding of the eigenvalues and the eigenfunctions of the perturbed self-adjoint operators is important for both applied mathematics and other fields of basic research. In this regard, the establishment of new and development of existing numerical methods for solving of spectral problems generated by perturbation discrete operators, are an actual problems of modern mathematical modeling of different processes of nature.

A new method was developed in the works, which were written by S.I. Kadchenko, together with academician V.A. Sadovnichii and professor V.V. Dubrovskii. This method allows to calculate the first eigenvalues of perturbed self-adjoint operators and was called the method of regularized traces (RT). Later, S.I. Kadchenko got very simple formulas for calculating of eigenvalues of perturbation discrete operators and removed a number of strong restrictions on the unperturbed and perturbing operators [1]. It greatly increased the computational effectiveness and greatly expanded the class of operators to which the method can be applied. S.I. Kadchenko and S.N. Kakushkin developed the ideas of the method of regularized traces. As a result, a non-iterative method, which allows to find the values of eigenfunctions of perturbed discrete operators in discrete nodes of the domain of definition, was developed [2–4]. The main theorems, which are used in the construction

of this method, are presented in this paper. Also formulas, which allow to calculate the values of sums of functional series of "suspended" corrections of perturbation theory of discrete operators, were obtained, and computational experiment was performed.

Let  $T$  be a discrete lower semibounded operator, and  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$  with domains of definition in  $D$ . Suppose that the eigenvalues  $\{\lambda_n\}_{n=1}^{\infty}$  of operator  $T$  are known and are numbered in decreasing order of their values. Also suppose that the orthonormal eigenfunctions  $\{v_n(x)\}_{n=1}^{\infty}$  ( $x \in D$ ), corresponding to these eigenvalues, are known and form a basis in  $H$ . Let  $\nu_n$  be algebraic multiplicity of the eigenvalue  $\lambda_n$ . Denote a number of unequal to each other  $\lambda_n$ , lying inside the circle  $T_{n_0}$ , having radius  $\rho_{n_0} = \frac{|\lambda_{n_0+1} + \lambda_{n_0}|}{2}$  and a centre at the origin of the complex plane, by  $n_0$ . Let  $\{\mu_n\}_{n=1}^{\infty}$  be eigenvalues of the operator  $T + P$ , which are numbered in not decreasing order of their real parts, and  $\{u_n(x)\}_{n=1}^{\infty}$  ( $x \in D$ ) be corresponding eigenfunctions.

The following theorem was obtained in paper [5].

**Theorem 1.** *Let  $T$  be a discrete lower semibounded operator, and  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$  with domains of definition in  $D$ . If the inequalities  $q_n = \frac{2\|P\|}{|\lambda_{n+\nu_n} - \lambda_n|} < 1$  are hold for all  $n \in \mathbb{N}$ , then  $m_0 = \sum_{n=1}^{n_0} \nu_n$  eigenfunctions of the operator  $T + P$  are the solutions of system of nonlinear equations*

$$\sum_{j=1}^{m_0} \mu_j^p u_j(x) \bar{u}_j(y) = \sum_{j=1}^{m_0} \lambda_j^p v_j(x) \bar{v}_j(y) + \sum_{k=1}^t \alpha_k^{(p)}(m_0, x, y) + \varphi_t^{(p)}(m_0, x, y). \quad (1)$$

Here

$$\alpha_k^{(p)}(m_0, x, y) = \frac{(-1)^k}{2\pi i} \int_{T_{n_0}} \lambda^p [K_T(x, z_k, \lambda) \circ P_{z_k}]^k \circ K_T(z_k, y, \lambda) d\lambda$$

are  $k$ -th corrections of perturbation theory to the "suspended" spectral function of the operator  $T + P$  of integer order  $p$ ;

$$\begin{aligned} \varphi_t^{(p)}(m_0, x, y) &= \frac{(-1)^{t+1}}{2\pi i} \int_{T_{n_0}} \lambda^p [K_T(x, z_{t+1}, \lambda) \circ P_{z_{t+1}}]^{t+1} \circ \\ &\quad \circ K_{T+P}(z_{t+1}, y, \lambda) d\lambda; \end{aligned}$$

operation " $\circ$ " is introduced by the rule

$$(K \circ P \circ Q)(x, y, \lambda) = \int_D K(x, z, \lambda) P_z Q(z, y, \lambda) dz; \quad (2)$$

$K_T(x, y, \lambda)$  – kernel of the resolvent  $R_\lambda(T)$  of operator  $T$ ;  $T_{n_0}$  – circle having radius  $\rho_{n_0} = \frac{|\lambda_{n_0+1} + \lambda_{n_0}|}{2}$  and centre at the origin of the complex plane.

It can be shown (using, for example, [6, chapter V, § 4, p. 331]), that  $|\varphi_t^{(p)}(m_0, x, y)| \rightarrow 0$  for  $m_0 \rightarrow \infty$ . Then the system of equations (1) becomes:

$$\sum_{j=1}^{m_0} \mu_j^p u_j(x) \bar{u}_j(y) = \sum_{j=1}^{m_0} \lambda_j^p v_j(x) \bar{v}_j(y) + \sum_{k=1}^t \alpha_k^{(p)}(m_0, x, y) + \varepsilon_t^{(p)}(m_0, x, y), \quad (3)$$

where

$$\varepsilon_t^{(p)}(m_0, x, y) = \sum_{k=t+1}^{\infty} \alpha_k^{(p)}(m_0, x, y).$$

The system of equations (3) is the basis of a new non-iterative numerical method of finding of the values of the eigenfunctions  $u_j(x)$  of perturbed operator  $T + P$  at the nodes of the sampling.

## 1. The RT Method to Calculate the Values of Eigenfunctions of Perturbed Discrete Operators

The difficulty of using of the system of equations (3) to calculate the values of products of  $u_j(x)\bar{u}_j(y)$  is to find sums of "suspended" corrections of perturbation theory  $\sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y)$ , which can be find only numerically. The estimates of "suspended" corrections of perturbation theory were obtained by analytical formulas.

**Theorem 2.** *Let  $T$  be a discrete lower semibounded operator, and  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$ . If the inequalities  $q_n < 1$  are hold for all  $n \in \mathbb{N}$ , then for "suspended" corrections of perturbation theory  $\alpha_m^{(p)}(m_0, x, y)$  of operator  $T + P$  the following estimates are true:*

$$|\alpha_m^{(p)}(m_0, x, y)| \leq \frac{C_0^2}{2\pi} \|P\| \rho_{n_0}^{p+1} q_{n_0}^{m-1} S_\lambda. \quad (4)$$

Here  $S_\lambda = \sup_{\lambda \in T_{n_0}} \left( \sum_{k=1}^{\infty} \frac{1}{|\lambda - \lambda_k|} \right)^2$ ,  $|v_i(x)| \leq C_0$ ,  $\forall i = \overline{1, \infty}$ .

The convergence of sums of Rayleigh – Schrodinger functional series  $\sum_{m=1}^{\infty} \alpha_m^{(p)}(m_0, x, y)$  is proved in paper [7] using (4). There the estimates of them were obtained.

**Theorem 3.** *Let  $T$  be a discrete lower semibounded operator, and  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$ . If the inequalities  $q_n < 1$  are hold for all  $n \in \mathbb{N}$ , then for sum remainders of Rayleigh – Schrodinger functional series  $\varepsilon_t^{(p)}(m_0, x, y)$  of operator  $T + P$  for any  $t, p, m_0 \in \mathbb{N}$  the following estimates are true:*

$$|\varepsilon_t^{(p)}(m_0, x, y)| \leq \frac{C_0^2}{2\pi} \|P\| \rho_{n_0}^{p+1} S_\lambda \frac{q_{n_0}^t}{1 - q_{n_0}}. \quad (5)$$

Here  $S_\lambda = \sup_{\lambda \in T_{n_0}} \left( \sum_{k=1}^{\infty} \frac{1}{|\lambda - \lambda_k|} \right)^2$ ,  $|v_i(x)| \leq C_0$ ,  $i = \overline{1, \infty}$ .

If the norm of the perturbing operator  $P$  is small, then it is enough to approach the sum of functional series  $\sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y)$  by the first "suspended" corrections. The limiting absolute errors of finding sums of functional series  $\sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y)$  are evaluated by the formulas (5). In the following theorem we obtain formulas for finding the "suspended" corrections of theory of perturbations  $\alpha_k^{(p)}(m_0, x, y)$  of discrete operators, such that one can

find approximately the sum of Rayleigh – Schrodinger functional series  $\sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y)$  by summing up them.

**Theorem 4.** *Let  $T$  be a discrete lower semibounded operator,  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$ . Suppose the inequalities  $q_n < 1$  are true for all  $n \in \mathbb{N}$ . Then the "suspended" corrections of theory of perturbations  $\alpha_k^{(p)}(m_0, x, y)$  for any natural  $k, p$  and  $m_0$  can be find by the formulas:*

$$\begin{aligned} \alpha_k^{(p)}(m_0, x, y) = & - \sum_{n=1}^{m_0} \sum_{j_1, \dots, j_{k+1}=1}^{\infty} v_{j_1}(x) \bar{v}_{j_{k+1}}(y) \times \\ & \times r_k^{(p)}(n, j_1, \dots, j_{k+1}) \prod_{m=1}^k V_{j_m j_{m+1}}, \end{aligned} \quad (6)$$

where

$$r_k^{(p)}(n, j_1, \dots, j_{k+1}) = \begin{cases} 0, & \forall j_m \neq n, m = \overline{1, k+1}; \\ \frac{1}{k!} \lim_{\lambda \rightarrow \lambda_n} \frac{d^k}{d\lambda^k} \lambda^p, & l = k+1; \\ \frac{1}{(l-1)!} \lim_{\lambda \rightarrow \lambda_n} \frac{d^{l-1}}{d\lambda^{l-1}} \left( \frac{\lambda^p}{\prod_{m=1}^{k-l+1} (\lambda - \lambda_{j_m})} \right), & 0 < l \leq k; \end{cases}$$

$V_{i,j} = (Pv_i, v_j)$  – inner product;  $l$  – number of coincidences  $j_m = n, m = \overline{1, k+1}$ .

The main determinant of the system of equations (1) is a Vandermonde determinant, and is different from zero. Therefore one can find its solution, with respect to products of  $u_j(x) \bar{u}_j(y)$ , by any appropriate method [5]. In the future, it is assumed that the eigenvalues  $\mu_n$  are found by new RS method, which was obtained by S.I. Kadchenko in papers [1, 9].

The technique of finding the values of products of eigenfunctions  $u_j(x) \bar{u}_j(y)$  of operators  $T + P$  is presented in the following theorem. This technique uses linear formulas of calculation and allows do not direct solve a system of nonlinear equations (3).

**Theorem 5.** *Let  $T$  be a discrete lower semibounded operator,  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$  with domain of definition  $D$ . Suppose the inequalities  $q_n < 1$  are true for all  $n \in \mathbb{N}$ . Then the value of the product of eigenfunction  $u_n(x)$  and its conjugate one  $\bar{u}_n(y)$  for all values of the arguments  $x, y \in D$ , can be find by the formulas:*

$$\begin{aligned} u_n(x) \bar{u}_n(y) = & \frac{1}{\mu_n} \left( \lambda_n v_n(x) \bar{v}_n(y) + \right. \\ & \left. + \sum_{k=1}^t [\alpha_k^{(1)}(n, x, y) - \alpha_k^{(1)}(n-1, x, y)] \right) + \tilde{\varepsilon}_t^{(1)}(n, x, y), \end{aligned} \quad (7)$$

where for  $\tilde{\varepsilon}_t^{(1)}(n, x, y)$  the estimates

$$|\tilde{\varepsilon}_t^{(1)}(n, x, y)| \leq \frac{C_0^2}{2\pi\mu_n} \|P\| S_\lambda \rho_n^2 \frac{q^t}{1-q}, \quad \forall t \in \mathbb{N}, n = \overline{1, m_0} \text{ are true.} \quad (8)$$

Here  $S_\lambda = \sup_{\lambda \in T_{n_0}} \left( \sum_{k=1}^{\infty} \frac{1}{|\lambda - \lambda_k|} \right)^2$ ,  $|v_i(x)| \leq C_0 \quad \forall i = \overline{1, \infty}$ ,  $q = \max_{n \geq 1} q_n$ .

In general, the values of the eigenfunctions of a perturbed self-adjoint operator are complex. The product of eigenfunction  $u_j(x)$  ( $j = \overline{1, m_0}$ ) and its conjugate one  $\bar{u}_j(x)$  at the same point  $x \in D$  is the module of values of eigenfunction  $u_j(x)$ . Therefore, one can not to restore the value of eigenfunction  $u_j(x)$  by one point using the equation (3). But if we consider the equation (3) for different points  $x$  and  $y$ , then it is possible to construct an algorithm for calculating the values of eigenfunctions.

Let us illustrate this for the case where the eigenfunctions  $\{u_n(x)\}_{n=1}^{m_0}$  of operator  $T + P$  are functions of  $k$  variables:  $x = (x_1, x_2, \dots, x_k)$ . We introduce the difference grid for arguments  $x_1, x_2 \dots x_k$  with steps  $h_1, h_2 \dots h_k$  respectively. Denote the number of nodes of the arguments  $x_1, x_2 \dots x_k$  by  $m_1, m_2 \dots m_k$ . Let us write the values  $x \in D$  at the nodes of a sample in the form

$$x_{j_1 j_2 \dots j_k} = (x_{1j_1}, x_{2j_2}, \dots, x_{kj_k}), \quad j_l = \overline{1, m_l}, \quad l = \overline{1, k}.$$

Denote the right side (7) by  $\varphi_n(x, y)$ . Then in the sampling nodes they take the form

$$u_n(x_{i_1 i_2 \dots i_k}) \bar{u}_n(y_{j_1 j_2 \dots j_k}) = \varphi_n(x_{i_1 i_2 \dots i_k}, y_{j_1 j_2 \dots j_k}), \quad (9)$$

where  $i_l, j_l = \overline{1, m_l}, l = \overline{1, k}$ .

Fix  $k - 1$  coordinates of the sampling points and write the equation (9) for two node points with coordinates  $x_{i_1 i_2 \dots i_k}, x_{i_1 i_2 \dots i_k}$  and  $x_{i_1 i_2 \dots i_k + 1}, x_{i_1 i_2 \dots i_k}$

$$u_n(x_{i_1 i_2 \dots i_k + 1}) \bar{u}_n(x_{i_1 i_2 \dots i_k}) = \varphi_n(x_{i_1 i_2 \dots i_k + 1}, x_{i_1 i_2 \dots i_k}).$$

First step is to find up to the sign the values of real and imaginary parts of  $u_n(x_{i_1 i_2 \dots i_k + 1})$  in the following form:

$$u_n(x_{i_1 i_2 \dots i_k + 1}) = \pm \frac{\varphi_n(x_{i_1 i_2 \dots i_k + 1}, x_{i_1 i_2 \dots i_k})}{\sqrt{\varphi_n(x_{i_1 i_2 \dots i_k}, x_{i_1 i_2 \dots i_k})}}, \quad i_k = \overline{1, m_k - 1}. \quad (10)$$

Similarly, we find the value of the eigenfunction  $u_n$  in the rest of the node points.

Let us determine the sign within the grid for each value  $u_n(x_{i_1 i_2 \dots i_k})$ , which was founded by the formulas (10).

Second step is to determine the sign of the founded values. To this end fix  $k - 2$  values of coordinates of grid points (in the description of the algorithm, to be specific, fix the first  $k - 2$  index) and consider the product of the form

$$u_n(x_{i_1 i_2 \dots i_{k-1}, i_k}) \bar{u}_n(x_{i_1 i_2 \dots i_{k-1}, i_k + 1}) \quad (11)$$

and

$$u_n(x_{i_1 i_2 \dots, i_{k-1}, i_k}) \bar{u}_n(x_{i_1 i_2 \dots, i_{k-1} + 1, i_k}). \quad (12)$$

Obviously, if the real part of the product (11) is negative, then values of function  $u_n$  have different signs in the points  $x_{i_1 i_2 \dots, i_{k-1}, i_k}$  and  $x_{i_1 i_2 \dots, i_{k-1}, i_k + 1}$ . Therefore, one can determine the change in the signs of values of eigenfunctions by looking at the values of the real part of the products at each node.

Introduce an auxiliary coefficient  $\xi$ , which is equal 1 or  $-1$ . For all  $i_k = 1$  the value  $\xi$  is set to be  $-1$ . We consider a sign of the product (12) at each sampling node and multiplie a modules of values  $u_n(x_{i_1 i_2 \dots i_{k-1} + 1, i_k})$  by  $\xi$ . If the real part of the product (12) is negative, then the sign of the coefficient  $\xi$  is reversed.

We carry out the same operations for the product (12). To not change the already changed in the previous step signs of values  $u_n(x_{i_1 i_2 \dots i_{k-1}, i_k})$  for  $i_{k-1} = 1$  set  $\xi = 1$ .

After the end of the described operations, we consider the coordinates of the remaining node points, increasing the values of fixed index  $i_1, i_2, \dots, i_{k-2}$  in turn by one.

RT method algorithm composed by the above-described scheme is presented in [8].

In the following theorem we obtain formulas that are convenient to find the sums of functional series of "suspended" corrections of perturbation theory  $\sum_{n=1}^{\infty} \alpha_n^{(p)}(m_0, x, y)$ .

**Theorem 6.** *Let  $T$  be a discrete lower semibounded operator, and  $P$  be bounded operator, and both are set in a separable Hilbert space  $H$  with domain of definition in  $D$ . If the functions  $\{v_n(x)\}_{n=1}^{\infty}$  ( $x \in D$ ) form an orthonormal basis in  $H$ , then the sums of functional series of "suspended" perturbation theory corrections are found by the formulas*

$$\begin{aligned} \sum_{n=1}^{\infty} \alpha_n^{(p)}(m_0, x, y) &= \sum_{k=1}^{m_0} \left[ \mu_k^p v_m(x) \bar{v}_m(y) - \lambda_k^p v_k(x) \bar{v}_k(y) - \right. \\ &- \mu_k^p \sum_{j,i=1}^{m-1} \left\{ \frac{\bar{V}_{im} \check{A}_{ij}^{(k)}}{\det \check{\mathbf{A}}^{(k)}} v_m(x) \bar{v}_j(y) + \frac{V_{im} \check{A}_{ij}^{(k)}}{\det \check{\mathbf{A}}^{(k)}} v_j(x) \bar{v}_m(y) \right\} + \\ &+ \mu_k^p \sum_{j_1, j_2, i_1, i_2=1}^{m-1} \frac{V_{i_1 m} \bar{V}_{i_2 m} \check{A}_{i_1 j_1}^{(k)} \overline{\check{A}_{i_2 j_2}^{(k)}}}{\det \check{\mathbf{A}}^{(k)} \det \check{\mathbf{A}}^{(k)}} v_{j_1}(x) v_{j_2}(y) \left. \right] + \delta_m^{(p)}(m_0, x, y). \end{aligned} \tag{13}$$

Here

$$\begin{aligned} \left| \delta_m^{(p)}(m_0, x, y) \right| &\leq \sum_{k=1}^{m_0} |\mu_k|^p \left[ 2|C| \cdot |\varepsilon_k^{(m)}| \sum_{j=1}^m |x_j^{(k)}| + |\varepsilon_k^{(m)}|^2 \right], \\ x_l^{(k)} &= \begin{cases} -\frac{1}{\det \check{\mathbf{A}}^{(k)}} \sum_{i=1}^{m-1} V_{im} \check{A}_{il}^{(k)}, & l = \overline{1, m-1}; \\ 1, & l = m. \end{cases} \end{aligned}$$

$C = \max_{i=1, m} |v_i(x)|$ ,  $|\delta_m^{(p)}(m_0, x, y)| \xrightarrow{m \rightarrow \infty} 0$ ,  $\varepsilon_k^{(m)} = u_k(x) - u_k^{(m)}(x)$ ,  $u_k^{(m)}(x)$  - approximation of the eigenfunction  $u_k(x)$ ,  $\check{\mathbf{A}}^{(k)} = (a_{ij})_{i,j=1}^m$ ,  $m \in \mathbb{N}$ ,  $a_{ij} = V_{ij} + (\lambda_i - \mu_k) \delta_{ij}$ ,  $V_{ij} = (Pv_i, v_j)$ ,  $\delta_{ij}$  - Kronecker symbol,  $\check{A}_{ij}^{(k)}$  - cofactors to the matrix entries  $\check{\mathbf{A}}^{(k)}$ . The bar denotes complex conjugation.

*Proof.*

Let the system of eigenfunctions  $\{v_n(x)\}_{n=1}^{\infty}$  of operator  $T$  form an orthonormal basis in  $H$ . Then the eigenfunctions  $u_k(x)$  of operator  $T + P$  can be represented as

$$u_k(x) = \sum_{i=1}^{\infty} c_i^{(k)} v_i(x). \tag{14}$$

Let  $\varepsilon_k^{(m)} = u_k(x) - u_k^{(m)}(x)$ , where  $u_k^{(m)}(x)$  -  $m$ -th partial sum of functional series (14).

Transform entries of the matrix  $\mathbf{A}_{m \times m} = (a_{ij})_{i,j=1}^m$ , where  $a_{ij} = ((T + P)v_i, v_j)$ . By the equations  $Tv_n = \lambda_n v_n$  and orthonormal system of functions  $\{v_n\}_{n=1}^{\infty}$  one can write the chain of equalities:

$$a_{ij} = ((T + P)v_i, v_j) = (Tv_i, v_j) + (Pv_i, v_j) =$$

$$= (\lambda_i v_i, v_j) + (Pv_i, v_j) = \lambda_i (v_i, v_j) + (Pv_i, v_j) = \lambda_i \delta_{ij} + V_{ij},$$

где  $\delta_{ij} = \begin{cases} 1, & i = j, \\ 0, & i \neq j \end{cases}$  – Kronecker delta,  $i, j = \overline{1, m}$ ,  $m \in \mathbb{N}$ .

An eigenvector  $\mathbf{X}_k^{(m)} = (x_1^{(k)}, x_2^{(k)}, \dots, x_m^{(k)})^T$  of matrix  $\mathbf{A}_{m \times m}$  ( $k = \overline{1, m}$ ), corresponding to an eigenvalue  $\mu_k$ , must satisfy the matrix equation:

$$(\mathbf{A}_{m \times m} - \mu_k \mathbf{E}) \mathbf{X}_k^{(m)} = 0$$

или

$$\begin{cases} (a_{11} - \mu_k)x_1^{(k)} + a_{12}x_2^{(k)} + \dots + a_{1m}x_m^{(k)} = 0; \\ a_{21}x_1^{(k)} + (a_{22} - \mu_k)x_2^{(k)} + \dots + a_{2m}x_m^{(k)} = 0; \\ \dots \\ a_{m1}x_1^{(k)} + a_{m2}x_2^{(k)} + \dots + (a_{mm} - \mu_k)x_m^{(k)} = 0. \end{cases} \quad (15)$$

An eigenvector  $\mathbf{X}_k^{(m)}$  is defined up to a factor. Therefore, let component  $x_m^{(k)}$  of vector  $\mathbf{X}_k^{(m)}$  be equal to unity. Discard the last of the equations of the system (15). Note that the remaining equations are linearly independent. The resulting system of equations can be presented in matrix form:

$$\begin{aligned} & \check{\mathbf{A}}^{(k)} \begin{pmatrix} x_1^{(k)} \\ x_2^{(k)} \\ \dots \\ x_{m-1}^{(k)} \end{pmatrix} = \mathbf{B} \sim \\ & \sim \begin{pmatrix} a_{11} - \mu_k & a_{12} & \dots & a_{1,m-1} \\ a_{21} & a_{22} - \mu_k & \dots & a_{2,m-1} \\ \dots & \dots & \dots & \dots \\ a_{m-1,1} & a_{m-1,2} & \dots & a_{m-1,m-1} - \mu_k \end{pmatrix} \begin{pmatrix} x_1^{(k)} \\ x_2^{(k)} \\ \dots \\ x_{m-1}^{(k)} \end{pmatrix} = \begin{pmatrix} -a_{1m} \\ -a_{2m} \\ \dots \\ -a_{m-1,m} \end{pmatrix}. \end{aligned} \quad (16)$$

From the form of a matrix  $\mathbf{A}_{m \times m} - \mu_k \mathbf{E}$  it is followed that  $a_{im} = V_{im}$ ,  $i = \overline{1, m-1}$ .

We solve heterogeneous system of equations (16) by the inverse matrix method:

$$\begin{aligned} & \begin{pmatrix} x_1^{(k)} \\ x_2^{(k)} \\ \dots \\ x_{m-1}^{(k)} \end{pmatrix} = [\check{\mathbf{A}}^{(k)}]^{-1} \mathbf{B} = \\ & = \frac{1}{\det \check{\mathbf{A}}^{(k)}} \begin{pmatrix} \check{A}_{11}^{(k)} & \check{A}_{21}^{(k)} & \dots & \check{A}_{m-1,1}^{(k)} \\ \check{A}_{12}^{(k)} & \check{A}_{22}^{(k)} & \dots & \check{A}_{m-1,2}^{(k)} \\ \dots & \dots & \dots & \dots \\ \check{A}_{1,m-1}^{(k)} & \check{A}_{2,m-1}^{(k)} & \dots & \check{A}_{m-1,m-1}^{(k)} \end{pmatrix} \begin{pmatrix} -V_{1m} \\ -V_{2m} \\ \dots \\ -V_{m-1,m} \end{pmatrix} = \\ & = \frac{1}{\det \check{\mathbf{A}}^{(k)}} \begin{pmatrix} -\sum_{i=1}^{m-1} V_{im} \check{A}_{i1}^{(k)} \\ -\sum_{i=1}^{m-1} V_{im} \check{A}_{i2}^{(k)} \\ \dots \\ -\sum_{i=1}^{m-1} V_{im} \check{A}_{i,m-1}^{(k)} \end{pmatrix}. \end{aligned}$$

Here  $\check{A}_{ij}^{(k)}$  – algebraic complements of entries of the matrix  $\check{\mathbf{A}}^{(k)}$  ( $i, j = \overline{1, m-1}$ ).

Therefore, components of the vector  $\mathbf{X}_k^{(m)}$  ( $k = \overline{1, m}$ ) take the form

$$x_l^{(k)} = \begin{cases} -\frac{1}{\det \check{\mathbf{A}}^{(k)}} \sum_{i=1}^{m-1} V_{im} \check{A}_{il}^{(k)}, & l = \overline{1, m-1}; \\ 1, & l = m. \end{cases} \quad (17)$$

Solve a system of equations (3) on  $\sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y)$ :

$$\begin{aligned} \sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y) &= \sum_{k=1}^{m_0} \left[ \mu_k^p u_k(x) \bar{u}_k(y) - \lambda_k^p v_k(x) \bar{v}_k(y) \right] = \\ &= \sum_{k=1}^{m_0} \left[ \mu_k^p \left( u_k^{(m)}(x) + \varepsilon_k^{(m)} \right) \left( \bar{u}_k^{(m)}(y) + \bar{\varepsilon}_k^{(m)} \right) - \lambda_k^p v_k(x) \bar{v}_k(y) \right] = \\ &= \sum_{k=1}^{m_0} \left\{ \mu_k^p \left[ u_k^{(m)}(x) \bar{u}_k^{(m)}(y) + \bar{\varepsilon}_k^{(m)} u_k^{(m)}(x) + \varepsilon_k^{(m)} \bar{u}_k^{(m)}(y) + \varepsilon_k^{(m)} \bar{\varepsilon}_k^{(m)} \right] - \lambda_k^p v_k(x) \bar{v}_k(y) \right\} = \\ &= \sum_{k=1}^{m_0} \left[ \mu_k^p u_k^{(m)}(x) \bar{u}_k^{(m)}(y) - \lambda_k^p v_k(x) \bar{v}_k(y) \right] + \sum_{k=1}^{m_0} \mu_k^p \left[ \bar{\varepsilon}_k^{(m)} u_k^{(m)}(x) + \varepsilon_k^{(m)} \bar{u}_k^{(m)}(y) + \varepsilon_k^{(m)} \bar{\varepsilon}_k^{(m)} \right] = \\ &= \sum_{k=1}^{m_0} \left[ \mu_k^p u_k^{(m)}(x) \bar{u}_k^{(m)}(y) - \lambda_k^p v_k(x) \bar{v}_k(y) \right] + \delta_m^{(p)}(m_0, x, y). \end{aligned}$$

Decompose the components of the eigenvector  $\mathbf{X}_k^{(m)}$  on the elements of an orthonormal basis  $\{v_i(x)\}_{i=1}^m$  ( $x \in D$ ), using formulas (17):

$$u_k^{(m)}(x) = \sum_{j=1}^m x_j^{(k)} v_j(x) = v_m(x) - \frac{1}{\det \check{\mathbf{A}}^{(k)}} \sum_{j=1}^{m-1} \sum_{i=1}^{m-1} V_{im} \check{A}_{ij}^{(k)} v_j(x). \quad (18)$$

Substitute formulas (18) in term for  $\sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y)$ :

$$\begin{aligned} \sum_{k=1}^{\infty} \alpha_k^{(p)}(m_0, x, y) &= \sum_{k=1}^{m_0} \left[ \mu_k^p \left( v_m(x) - \frac{1}{\det \check{\mathbf{A}}^{(k)}} \sum_{j,i=1}^{m-1} V_{im} \check{A}_{ij}^{(k)} v_j(x) \right) \times \right. \\ &\quad \left. \times \left( \bar{v}_m(y) - \frac{1}{\det \check{\mathbf{A}}^{(k)}} \sum_{j,i=1}^{m-1} \bar{V}_{im} \check{A}_{ij}^{(k)} \bar{v}_j(y) \right) - \lambda_k^p v_k(x) \bar{v}_k(y) \right] + \delta_m^{(p)}(m_0, x, y) = \\ &= \sum_{k=1}^{m_0} \left[ \mu_k^p \left\{ v_m(x) \bar{v}_m(y) - \frac{v_m(x)}{\det \check{\mathbf{A}}^{(k)}} \sum_{j,i=1}^{m-1} \bar{V}_{im} \check{A}_{ij}^{(k)} \bar{v}_j(y) - \frac{\bar{v}_m(y)}{\det \check{\mathbf{A}}^{(k)}} \sum_{j,i=1}^{m-1} V_{im} \check{A}_{ij}^{(k)} v_j(x) + \right. \right. \\ &\quad \left. \left. + \sum_{j_1, j_2, i_1, i_2=1}^{m-1} \frac{V_{i_1 m} \bar{V}_{i_2 m} \check{A}_{i_1 j_1}^{(k)} \check{A}_{i_2 j_2}^{(k)}}{\det \check{\mathbf{A}}^{(k)} \det \check{\mathbf{A}}^{(k)}} v_{j_1}(x) v_{j_2}(y) \right\} - \lambda_k^p v_k(x) \bar{v}_k(y) \right] + \delta_m^{(p)}(m_0, x, y) = \end{aligned}$$



$$\begin{aligned}
 &= \sum_{k=1}^{m_0} \left[ \mu_k^p v_m(x) \bar{v}_m(y) - \lambda_k^p v_k(x) \bar{v}_k(y) - \mu_k^p \sum_{j,i=1}^{m-1} \left\{ \frac{\bar{V}_{im} \overline{\check{A}_{ij}^{(k)}}}{\det \check{\mathbf{A}}^{(k)}} v_m(x) \bar{v}_j(y) + \frac{V_{im} \check{A}_{ij}^{(k)}}{\det \check{\mathbf{A}}^{(k)}} v_j(x) \bar{v}_m(y) \right\} + \right. \\
 &\quad \left. + \mu_k^p \sum_{j_1, j_2, i_1, i_2=1}^{m-1} \frac{V_{i_1 m} \bar{V}_{i_2 m} \check{A}_{i_1 j_1}^{(k)} \overline{\check{A}_{i_2 j_2}^{(k)}}}{\det \check{\mathbf{A}}^{(k)} \det \check{\mathbf{A}}^{(k)}} v_{j_1}(x) v_{j_2}(y) \right] + \delta_m^{(p)}(m_0, x, y).
 \end{aligned}$$

We estimate residues  $|\delta_m^{(p)}(m_0, x, y)|$ :

$$\begin{aligned}
 \left| \delta_m^{(p)}(m_0, x, y) \right| &= \left| \sum_{k=1}^{m_0} \mu_k^p \left[ \bar{\varepsilon}_k^{(m)} u_k^{(m)}(x) + \varepsilon_k^{(m)} \bar{u}_k^{(m)}(y) + \varepsilon_k^{(m)} \bar{\varepsilon}_k^{(m)} \right] \right| \leq \\
 &\leq \sum_{k=1}^{m_0} |\mu_k|^p \left[ |C \bar{\varepsilon}_k^{(m)} \sum_{j=1}^m x_j^{(k)}| + |C \varepsilon_k^{(m)} \sum_{j=1}^m \bar{x}_j^{(k)}| + |\varepsilon_k^{(m)} \bar{\varepsilon}_k^{(m)}| \right] \leq \\
 &\leq \sum_{k=1}^{m_0} |\mu_k|^p \left[ 2|C| \cdot |\varepsilon_k^{(m)}| \sum_{j=1}^m |x_j^{(k)}| + |\varepsilon_k^{(m)}|^2 \right].
 \end{aligned}$$

Here  $C = \max_{i=1, m} |v_i(x)|$ , and  $x_j^{(k)}$  are calculated by formulas (17).

The theorem is proved. □

## 2. Computational Experiment

Let an operator  $T = -\Delta$  be defined on the interval  $D = [0, l]$ . As a perturbing operator  $P$  we take the operator of multiplication by function  $p(x)$ , defined on the interval  $D$ .

Consider the spectral problem

$$\begin{aligned}
 &(T + P)u = \mu u, \quad u \in D_T. \\
 D_T &= \left\{ u \mid u \in C^2(D) \cap C(D), \Delta u \in L_2[D] : u \Big|_0 = u \Big|_l = 0 \right\}.
 \end{aligned}$$

It is well known that eigenvalues  $\lambda_n$  and eigenfunctions  $v_n(x)$  of 1-dimensional Laplace operator have the form:

$$\lambda_n = \left( \frac{\pi n}{l} \right)^2, \quad v_n(x) = \sin(\sqrt{\lambda_n} x), \quad x \in D.$$

Using formulas (7) and (13) the values of the fifth and sixth of the eigenfunctions of the perturbed operator  $T + P$  were found. Tables 1 and 2 shows the values of the left and right sides of the equation  $(T + P)u_n = \mu_n u_n$ .

Table 3 shows the values of the residual  $\|(T + P)u_n - \mu_n u_n\|$  for the first 10 eigenfunctions  $u_n$  for different perturbing operator  $P$ .

**Table 1**

The values  $(T + P)u_5$  and  $\mu_5 u_5$  for a perturbed Laplace operator calculated for  $l = 1$  and  $p(x) = x^2$

$x_j$	$(T + P)u_5(x_j)$	$\mu_5 u_5(x_j)$	$ (T + P)u_5(x_j) - \mu_5 u_5(x_j) $	$\left  \frac{(T + P)u_5(x_j) - \mu_5 u_5(x_j)}{\mu_5 u_5(x_j)} \right  \times 100\%$
0, 142857	272, 83735198766	273, 18110548326	0, 34375	0, 125834
0, 285714	340, 30702671043	340, 65126665861	0, 34424	0, 101053
0, 428571	151, 51348751144	151, 60407602055	0, 09059	0, 059753
0, 571429	151, 60114526407	151, 60407602055	0, 00293	0, 001933
0, 714286	340, 89792225718	340, 65126665861	0, 24666	0, 072407
0, 857143	273, 62712104909	273, 18110548325	0, 44602	0, 163267

**Table 2**

The values  $(T + P)u_6$  and  $\mu_6 u_6$  for a perturbed Laplace operator calculated for  $l = 1$  and  $p(x) = \sin \frac{x}{3} + 1$

$x_j$	$(T + P)u_6(x_j)$	$\mu_6 u_6(x_j)$	$ (T + P)u_6(x_j) - \mu_6 u_6(x_j) $	$\left  \frac{(T + P)u_6(x_j) - \mu_6 u_6(x_j)}{\mu_6 u_6(x_j)} \right  \times 100\%$
0, 142857	218, 65994242645	218, 73206609730	0, 0721237	0, 0329735
0, 285714	394, 06411361875	394, 14156393128	0, 0774503	0, 0196504
0, 428571	491, 45509644760	491, 48649119961	0, 0313948	0, 0063877
0, 571429	491, 51983562427	491, 48649119961	0, 0333444	0, 0067844
0, 714286	394, 21974628211	394, 14156393128	0, 0781824	0, 0198361
0, 857143	218, 80367419419	218, 73206609730	0, 0716081	0, 0327378

**Table 3**

The values of the residual  $\|(T + P)u_n - \mu_n u_n\|$  for a perturbed Laplace operator calculated for  $l = 1, m = n$

$n$	$\ (T + P)u_n - \mu_n u_n\ $ for $p(x) = \sin \frac{x}{3} + 1$	$\ (T + P)u_n - \mu_n u_n\ $ for $p(x) = x^2$
1	0, 05933175453013449	0, 18486186946562712
2	0, 08722167298850077	0, 26982226399384459
3	0, 09141711850816346	0, 28555566913308841
4	0, 09283781270256698	0, 29106235945347709
5	0, 09348757188208574	0, 29361116877997433
6	0, 09383850642063260	0, 29499570545892765
7	0, 09404942961086482	0, 29583053561545063
8	0, 09418605494412680	0, 29637237064820354
9	0, 09427960126060587	0, 29674384907194357
10	0, 09434645249551450	0, 29700956347750404

## Conclusion

The paper presents the main theorems, which are used to substantiate the method of regularized traces of finding of the values of eigenfunctions of perturbed self-adjoint operators in the sample nodes. For the first time formulas, which allow to calculate the

values of sums of functional series of "suspended" corrections of perturbation theory of discrete operators, were obtained. Computational experiments are performed. These experiments allowed to determine the values of the eigenfunctions of the perturbed one-dimensional Laplace operator. The experimental results showed the accuracy and computational efficiency of the developed method.

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## ВЫЧИСЛЕНИЕ ЗНАЧЕНИЙ СОБСТВЕННЫХ ФУНКЦИЙ ВОЗМУЩЕННЫХ САМОСОПРЯЖЕННЫХ ОПЕРАТОРОВ МЕТОДОМ РЕГУЛЯРИЗОВАННЫХ СЛЕДОВ

*С.Н. Какушкин, С.И. Кадченко*

Авторами статьи был разработан итерационный численный метод нахождения значений собственных функций возмущенных самосопряженных операторов, названный методом регуляризованных следов. Он позволяет найти значения собственных функций возмущенных дискретных операторов, зная спектральные характеристики невозмущенного оператора и собственные числа возмущенного оператора. В отличие от известных методов, в методе регуляризованных следов значения собственных функций находятся по линейным формулам. Это значительно увеличивает вычислительную эффективность. Сложность применения метода заключается в нахождении сумм функциональных рядов "взвешенных" поправок теории возмущений, которые можно найти лишь численно. В работе приведены формулы, удобные для нахождения "взвешенных" поправок, суммируя которые можно приблизить суммы этих функциональных рядов. Однако, если норма возмущающего оператора велика, то суммирование "взвешенных" поправок бывает не эффективным. В работе получены аналитические формулы нахождения значений сумм функциональных рядов "взвешенных" поправок теории возмущений в узлах дискретизации без непосредственного суммирования его членов. Проведены вычислительные эксперименты по нахождению значений собственных функций возмущенного одномерного оператора Лапласа. Результаты эксперимента показали точность и вычислительную эффективность разработанного метода.

*Ключевые слова: метод регуляризованных следов; возмущенные операторы; собственные числа; собственные функции; кратный спектр; "взвешенные" поправки теории возмущений.*

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