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FD-METHOD FOR SOLVING THE STURM–LIOUVILLE PROBLEM WITH POTENTIAL THAT IS THE DERIVATIVE OF A FUNCTION OF BOUNDED VARIATION

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Резюме. Розглядається скалярна задача Штурма-Ліувілля з потенціалом, що є похідною від функції обмеженої варіації, та крайовими умовами Діріхле. Викладена основа реалізації FD-методу у випадку, коли функція $\bar{q}(x)$, що наближає потенціал $q(x)$, є тотожнім нулем, а також у загальному випадку. Встановлені достатні умови суперекспоненціальної збіжності FD-методу та оцінки його точності, які є значним посиленням та узагальненням відповідних результатів, отриманих в попередніх роботах.

Abstract. We consider a scalar Sturm-Liouville problem with the Dirichlet boundary conditions where the potential $q(x)$ is assumed to be a derivative of the function with bounded variation. The application of the abstract FD-method scheme to such eigenvalue problem is studied in the scope of this work. In addition to the general case when the function $\bar{q}(x)$ approximating $q(x)$ is assumed to be arbitrary we study the case when $\bar{q}(x)$ is equal to zero everywhere. We obtain new sufficient conditions for the super-exponential convergence of the FD-method and its accuracy estimates which essentially generalize similar results obtained in the earlier works.

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1. Introduction

Most of the current technological and industrial advancements in electronics rely on the increasingly rigorous quantum-mechanical models. The models where the discontinuities of the potential are essential to represent the modelled phenomena and can not be disregarded. Mathematically such models can be represented as follows (*the one particle, many center Hamiltonian*):

$$\mathcal{H} = -\Delta + \sum_{\alpha\in\aleph} \gamma_\alpha \delta_\alpha(\cdot), \tag{1}$$

where Δ is a Laplace operator in $L^2(R^d)$, d stands for the dimension of the configuration space, $\aleph$ is a discrete, countable at most, subset in R^d, $\delta_\alpha(\cdot)$ is a Dirac delta function at the point α (i.e. a single measure concentrated at α) (see [1]). $\mathcal{H}$ describes the energy of the quantum mechanical particle which moves under the influence of an "interaction potential" created by the "point source" forces γ_α, located at α. We will denote this function as $\delta(x)$ and refer to it as Dirac delta function (**DDF**).

Key words. Sturm-Liouville problem, Dirac delta function potential, distribution potential, functional-discrete method, super-exponential convergence rate.

Dirac delta function (DDF) *potentials* had been used for modelling of atomic and molecular systems including atomic lattices, quantum heterostructures, semiconductors, organic fluorescent materials, solar cells etc. (see [1, 2, 3] and citations of them). Among recent applications of (1) one may mention the novel structure of quantum waveguide [2] based on the modelling with the same potential as in (1) having the finite numbers of delta functions. This type of potentials are called *Dirac comb* by the authors of [2]. History of the studies, mathematical properties and the visualization for some of the models involving such discontinuous potentials as well as various physical applications are summarized in [3].

Linear Sturm-Liouville problem with *distribution potentials* are extensively studied theoretically (for example see [4]). The authors of [5] derive the total regularized trace formula of differential Sturm–Liouville operators on a finite closed interval with singular potentials $q(x)$ that are not locally integrable functions and such that $\int q(x)dx \in BV_c[0,\pi]$ in the sense of distributions (the definition of $BV_c[0,\pi]$ will be given shortly). During the technical revision of [5] author of [6] found a simple proof for the case of potential $q(x) = \delta\left(x - \frac{\pi}{2}\right)$. Note that if $q(x) \in L_1$ then Theorem 1 from [5] contains the results of [7]. Independently from [5] the authors of [8] received the spectral asymptotic and the trace formula on the interval $[0, l]$ for the class of potentials, which may contain finite of sum δ-functions.

In the current paper we study an eigenvalue problem for the Hamiltonian having the form (1) with $d = 1$, $\aleph = \{\alpha\}$, $\alpha \in (0, 1)$, which is stated as follows:

$$\frac{d^2u(x)}{dx^2} + (\lambda - q(x))\,u(x) = 0,\ x \in (0,1),\ u(0) = 0,\ u(1) = 0, \tag{2}$$

where

$$q(x) = \frac{d\sigma(x)}{dx}$$

and $\sigma(x)$ is a function of bounded variation.

We start by summarizing some useful facts from the real analysis. Since $\sigma(x)$ is the function of bounded variation, the following representation is valid:

$$\sigma(x) = h(x) + \psi(x) + \chi(x),$$

with $h(x)$, $\psi(x)$, $\chi(x)$ being the jump function, the absolutely continuous function and the singular function correspondingly (see. [9], p.347). The singular part $\chi(x)$ has at most countable number of discontinuities which coincide with those of the jump function $h(x)$. Let us enumerate these discontinuity points in the ascending order and denote them as $x_p \in (0, 1)$, $p = 1, 2, \ldots$, $x_1 < x_2 < \ldots$, then $h(x) = \sum_p \gamma_p H(x - x_p)$, where γ_p are real numbers, $H(z)$ is the Heaviside function. From now on we assume that $\sigma(x)$ belongs to the class $BV_c[0, 1]$. That is the class of functions with bounded variation and which are right continuous at any point $x \in (0, 1)$ and continuous at the endpoints $x = 0$ and $x = 1$.

An essential role in the proof of FD-method's convergence rely on the following result:

Theorem 1. *([10], p.481) Let $\sigma(x) \in BV_c[0,1]$ and a function $f(x)$ be continuous on the segment $[0,1]$, then the following inequality holds true:*

$$\left| \int_0^1 f(x) d\sigma(x) \right| \le \max_{x \in [0,1]} |f(x)| \, \|\sigma\|_v ,$$

where $\|\sigma\|_v = \operatorname{var}\{\sigma(x); 0, 1\}$.

Due to the importance of the model there exist a large number of software packages for the numerical solution of the singular scalar Sturm-Liouville problems. Most notable FORTRAN packages are SL02F [11] and SLEDGE [12] implementing the Pruess method, SLEIGN [13, 14] and SLEIGN2 [15] – shooting method based on the Prüfer transformation. MATSLISE package [16] implements the Constant Perturbation Methods (CPM) and the Line Perturbation Methods (LPM) in MATLAB.

The code of SLEIGN2 became a considerable improvement of SLEIGN code. It covers more problem cases than other software packages, existent at that moment. Among other things the developers of SLEIGN2 expand the list of singular self-adjoint problems compatible with the package. Such list along with problem's classification, numerical examples and the package documentation can be found in [15]. The mentioned FORTRAN codes is available as a part of SLTSTPAK package (see [17]). Its implementation details as well as 60 test problem application examples are given [18]. Taking in to account the joint interest from different application areas, and the lack of common interface for the mentioned software packages the developers (V. Ledoux and rest of authors) created MATSLISE. It offers an interactive graphical user interface for various Sturm-Liouville problem solvers and the ability to control the parameters of the solver on-the-fly. Aside of that it contains some useful solution visualization tools (see [19]).

In spite of the large amount of implementations none of the mentioned packages can handle DDF potentials directly.

The purpose of the current work is to study, justify and propose algorithm implementation of the FD-method for eigenvalue problem for the Sturm-Liouville operator (2) with the potential being the derivative of the function with bounded variation such as

$$q(x) = \sum_{p=1}^{k} \gamma_p \delta(x - x_p) + \psi'(x), \; x_p \in (0,1), \; p = \overline{1,k}.$$

The results, presented here, extends the results reported in [20] in the linear case ($N(u) \equiv 0$), where the potential $q(x)$ have only one singularity ($k = 1$). Aside of that the current work contains the generalization of section 5 from [21], where the FD-method (with $\bar{q}(x) \equiv 0$) considered in application to (2) with $q(x) = a\delta\left(x - \frac{1}{2}\right), \; a > 0$.

In section 2 we apply the simplest version of the FD-method, when the function $\bar{q}(x)$, approximating the potential $q(x)$, is zero everywhere. The necessary conditions of the applied method's convergence is given. We show that under such conditions the method will converge super-exponentially. The practical implications of the technique proposed here lie in the fact that theoretical estimates on the lowest eigenvalue number for which the method is justified to converge, are more close to the number obtained experimentally. It may be considered as an improvement of the similar conditions from theorem 1 [8]. In the end of the section we present some numerical experiments to justify our theoretical results. The algorithm of general FD-method scheme ($\bar{q}(x) \not\equiv 0$) along with its justification is given in section 3. The results of a numerical calculation presented in the end of the section illustrate the effectiveness of the proposed algorithm.

2. FD-method for $\bar{q}(x) \equiv 0$

To find the approximate solution of the problem (2) we shall apply the FD-method of the m-th rank with the function $\bar{q}(x) \equiv 0$. Detailed justification for the choice of the FD-method scheme used here will be given in section 3 dealing with the general case $\bar{q}(x) \not\equiv 0$. The m-th rank approximate solution will be sought in the form of a finite sum

$$\overset{m}{u}_n(x) = \sum_{j=0}^{m} u_n^{(j)}(x), \ \overset{m}{\lambda}_n = \sum_{j=0}^{m} \lambda_n^{(j)}, \tag{3}$$

where every summand in (3) is obtained from the solution of the recurrent sequence of problems

$$\begin{gathered}\frac{d^2 u_n^{(j+1)}(x)}{dx^2} + \lambda_n^{(0)} u_n^{(j+1)}(x) = -\sum_{p=0}^{j} \lambda_n^{(j+1-p)} u_n^{(p)}(x) + q(x) u_n^{(j)}(x), \\ u_n^{(j+1)}(0) = 0, \ u_n^{(j+1)}(1) = 0, \ x \in (0,1), \ j = 0,1,...,m-1, \\ u_n^{(0)} = \sqrt{2}\sin(n\pi x), \ \lambda_n^{(0)} = (n\pi)^2,\end{gathered} \tag{4}$$

supplied by the solvability condition

$$\lambda_n^{(j+1)} = -\sum_{p=1}^{j} \lambda_n^{(j+1-p)} \int_0^1 u_n^{(p)}(x)\, u_n^{(0)}(x) dx + \int_0^1 q(x) u_n^{(j)}(x)\, u_n^{(0)}(x) dx$$

and the following orthogonality condition

$$\int_0^1 u_n^{(j+1)}(x)\, u_n^{(0)}(x) dx = 0,$$

which guaranties the uniqueness of the solution to (4). Let us represent the solution to (4) using the generalized Green's function approach:

$$u_n^{(j+1)}(x) = \int_0^1 g_n(x,\xi)\left[-\sum_{p=0}^{j}\lambda_n^{(j+1-p)}u_n^{(p)}(\xi)+q(\xi)u_n^{(j)}(\xi)\right]d\xi =$$

$$= -\sum_{p=0}^{j}\lambda_n^{(j+1-p)}\int_0^1 g_n(x,\xi)u_n^{(p)}(\xi)d\xi + \int_0^1 g_n(x,\xi)u_n^{(j)}(\xi)d\sigma(\xi), \quad (5)$$

$$\lambda_n^{(j+1)} = \int_0^1 q(\xi)u_n^{(j)}(\xi)u_n^{(0)}(\xi)d\xi = \int_0^1 u_n^{(j)}(\xi)u_n^{(0)}(\xi)d\sigma(\xi),$$

where

$$g_n(x,\xi) = \left[\frac{(x-H(x-\xi))\cos(n\pi x)}{\pi n} - \frac{\sin(n\pi x)}{2\pi^2 n^2}\right]\sin(n\pi\xi) +$$

$$+ \frac{\sin(n\pi x)(\xi - H(\xi - x))\cos(n\pi\xi)}{\pi n} = g_{n,1}(x,\xi) + g_{n,2}(x,\xi),$$

$$g_{n,1}(x,\xi) = \frac{(x-H(x-\xi))\cos(n\pi x)}{\pi n}\sin(n\pi\xi) + \quad (6)$$

$$+ \frac{\sin(n\pi x)(\xi-H(\xi-x))}{\pi n}\cos(n\pi\xi),$$

$$g_{n,2}(x,\xi) = -\frac{\sin(n\pi x)}{2\pi^2 n^2}\sin(n\pi\xi).$$

The generalized Green's function $g_n(x,\xi)$ has the following properties:

$$g_n(x,\xi) = g_n(\xi,x),\ g_n(x,\xi) = g_n(1-x,1-\xi),$$

$$\int_0^1 g_n(x,\xi)\sin(n\pi x)dx = 0,\ \int_0^1 g_n(x,\xi)\sin(n\pi\xi)d\xi = 0, \quad (7)$$

$$|g_n(x,\xi)| \le \frac{1}{\pi n} + \frac{1}{2(\pi n)^2} \le \frac{7}{6\pi n}.$$

Representation (5) along with the properties of Green function (7) and the results of theorem 1 allows us to obtain the following recurrent system of inequalities

$$\left\|u_n^{(j+1)}\right\|_\infty \le \|g_n\|_\infty\left(\sum_{p=1}^{j}\left|\lambda_n^{(j+1-p)}\right|\left\|u_n^{(p)}\right\|_\infty + \left\|u_n^{(j)}\right\|_\infty \|\sigma\|_v\right),$$

$$\left|\lambda_n^{(j+1)}\right| \le \sqrt{2}\left\|u_n^{(j)}\right\|_\infty \|\sigma\|_v, \quad (8)$$

$$j = 0,1,...,m-1.$$

One can deduce from (8) that

$$\left\|u_n^{(j+1)}\right\| \le M_n\sum_{p=0}^{j}\left\|u_n^{(j-p)}\right\|\left\|u_n^{(p)}\right\|_\infty,$$

where $M_n = \sqrt{2}\,\|g_n\|_\infty \|\sigma\|_v \le \sqrt{2}\frac{7}{6\pi n}\|\sigma\|_v$.

To obtain the solution of (8) we use the generating functions method (see [22]). It gives us the following sequence of estimates for the solution

$$\left\|u_n^{(j)}\right\|_\infty \le 2\sqrt{2}\frac{(2j-1)!!}{(2j+2)!!}(4M_n)^j \le \sqrt{2}\frac{(4M_n)^j}{(j+1)\sqrt{\pi j}},$$
$$\left|\lambda_n^{(j+1)}\right| \le 4\|\sigma\|_v \frac{(2j-1)!!}{(2j+2)!!}(4M_n)^j \le 2\|\sigma\|_v \frac{(4M_n)^j}{(j+1)\sqrt{\pi j}},$$
$$j = 0, 1, ..., m-1,$$

where $(2j)!! = 2 \cdot 4 \cdot ... \cdot 2j$, $(2j+1)!! = 1 \cdot 3 \cdot ... \cdot (2j+1)$. These estimates along with the assumptions regarding the form of $\sigma(x)$ yields the next result.

Theorem 2. *Let $\sigma(x) \in BV_c[0,1]$ and the following condition holds true*

$$r_n \overset{def}{=} 4M_n = 4\sqrt{2}\,\|g_n\|_\infty \|\sigma\|_v < 1, \tag{9}$$

then the FD-method for the Sturm–Liouville problem (2) converges super-exponentially. Moreover the error estimates satisfy (10), (11)

$$\left\|u_n - \overset{m}{u}_n\right\|_\infty = \left\|u_n - \sum_{j=0}^{m} u_n^{(j+1)}\right\|_\infty \le \frac{\sqrt{2}r_n^{m+1}}{(m+2)\sqrt{\pi(m+1)}(1-r_n)}, \tag{10}$$

$$\left|\lambda_n - \overset{m}{\lambda}_n\right| = \left|\lambda_n - \sum_{j=0}^{m} \lambda_n^{(j+1)}\right| \le \frac{2\|\sigma\|_v r_n^m}{(m+1)\sqrt{\pi m}(1-r_n)}. \tag{11}$$

This result is a considerable extension and generalization of the similar results of section 5 from [21], as well as the results of theorem 1 from [8]. In order to show that let us recall the similar result from [8]. If $\sigma(x) \in BV_c[0,1]$ and

$$n > \frac{1}{4\pi}\left(\frac{681}{16}\|\sigma\|_v + 1\right) \overset{def}{=} n_b \tag{12}$$

then the following representation (in the notation of current work) is valid

$$\lambda_n = (\pi n)^2 - \int_0^1 \left[u_n^{(0)}(x)\right]^2 d\sigma(x) - \int_0^1\int_0^1 k_n(\xi_1,\xi_2)d\sigma(\xi_1)d\sigma(\xi_2) + \nu'_{n,2}(\sigma),$$

where

$$k_n(\xi_1,\xi_2) \equiv \frac{1}{4\pi n}\sum_{i=1}^{2}(1-\cos(2\pi n\xi_i))\sin(2\pi n\xi_{3-i}) \times$$
$$\times \left[\frac{2}{\pi}\Theta(2\pi\xi_{3-i}) + (-1)^{i-1}sgn(\xi_2-\xi_1)\right],$$
$$\Theta(t) = (\pi - t)/2,$$

$$\left|\nu'_{n,2}(\sigma)\right| \le \|\sigma\|_v^2 \frac{4.4 + 467\|\sigma\|_v + 2\|\sigma\|_v^2}{\left(\pi n - \frac{1}{4}\right)^2} \overset{def}{=} \gamma_b(n, \|\sigma\|_v). \tag{13}$$

At the same time, it follows from theorem 2 that

$$\lambda_n = (\pi n)^2 + \lambda_n^{(1)} + \lambda_n^{(2)} + R_n^{(3)}, \tag{14}$$

where

$$\lambda_n^{(1)} = \int_0^1 \left[u_n^{(0)}(x)\right]^2 d\sigma(x),\ \lambda_n^{(2)} = \int_0^1 u_n^{(0)}(x) u_n^{(1)}(x) d\sigma(x),$$

$$u_n^{(1)}(x) = \int_0^1 g_n(x,\xi) u_n^{(0)}(\xi) d\sigma(\xi),$$

while the residual term $R_n^{(3)}$ satisfies

$$\left|R_n^{(3)}\right| \le \frac{2\left\|\sigma\right\|_v r_n^2}{3\sqrt{2\pi}(1-r_n)}, \tag{15}$$

as long as (9) holds. To make the comparison of the estimates (13) and (15) more convenient, we employ the estimate for r_n

$$r_n \overset{def}{=} 4\sqrt{2}\left\|g_n\right\|_\infty \left\|\sigma\right\|_v \le 4\sqrt{2}\left[\frac{1}{\pi n} + \frac{1}{2(\pi n)^2}\right]\left\|\sigma\right\|_v \overset{def}{=} r_{n,1} \le$$
$$\le \frac{14\sqrt{2}}{3\pi n}\left\|\sigma\right\|_v \overset{def}{=} r_{n,2}.$$

Then the estimate (15) could be replaced by the estimate

$$\left|R_n^{(3)}\right| \le \frac{2\left\|\sigma\right\|_v r_{n,1}^2}{3\sqrt{2\pi}(1-r_{n,1})} \overset{def}{=} \gamma_m\left(n, \left\|\sigma\right\|_v\right), \tag{16}$$

valid for all n such that

$$n > \frac{2\sqrt{2}}{\pi}\left(\left\|\sigma\right\|_v + \sqrt{\left\|\sigma\right\|_v^2 + \frac{\sqrt{2}}{4}\left\|\sigma\right\|_v}\right) \overset{def}{=} n_m. \tag{17}$$

By comparing (12) and (17) it is easy to see that

$$n_b > n_m,\ \forall \left\|\sigma\right\|_v \in [0,\infty),\ \lim_{\left\|\sigma\right\|_v \to \infty}(n_b - n_m) = \infty,$$

i.e. the condition (17) is less strict than the condition (12). Let us now compare estimates (16) and (13) for the residual terms for $n > n_b$, when both estimates make sense. For the clarity we remove the second summand from

$$\lambda_n^{(2)} = \int_0^1 u_n^{(0)}(x) \int_0^1 g_{n,1}(x,\xi) u_n^{(0)}(\xi) d\sigma(\xi) d\sigma(x) +$$
$$+ \int_0^1 u_n^{(0)}(x) \int_0^1 g_{n,2}(x,\xi) u_n^{(0)}(\xi) d\sigma(\xi) d\sigma(x) = \lambda_{n,1}^{(2)} + \lambda_{n,2}^{(2)}$$

(see (6)) and combine it with $R_n^{(3)}$. One can observe, afterwards, that

$$\nu'_{n,2}(\sigma) = R_n^{(3)} + \lambda_{n,2}^{(2)},$$

which after taking the norm of both sides lead us to the estimate for

$$\left|\nu'_{n,2}(\sigma)\right| \leq \left|R_n^{(3)}\right| + \left|\lambda_{n,2}^{(2)}\right| \leq \frac{2\left\|\sigma\right\|_v r_{n,1}^2}{3\sqrt{\pi}2(1-r_{n,1})} + \frac{\left\|\sigma\right\|_v^2}{(n\pi)^2} \stackrel{def}{=} \tilde{\gamma}_m(n, \left\|\sigma\right\|_v).$$

Using the elementary computations we see that

$$\gamma_b(n, \left\|\sigma\right\|_v) > \tilde{\gamma}_m(n, \left\|\sigma\right\|_v), \;\; \forall \left\|\sigma\right\|_v \geq 0.$$

Consequently, we have shown that the second-rank FD-method could be more efficient than the approach suggested in [21] from the accuracy standpoint.

Example 2.1. Let us consider problem (2) with the potential $q(x) = \delta(x-a)$ for $\bar{q}(x) \equiv 0$, where a is a real number and $a \in (0,1)$. The algorithm of FD method described above is *exactly realizable* (see [23]) in this case.

Let us denote

$$I_0(x) = g_n(t,a), \quad I_j(x) = \int_0^1 g_n(x,t)\, I_{j-1}(t)\, dt, \; j = 1, 2, \; \ldots .$$

By applying and the so-called *sifting* or *sampling property* for function $f \in C^1[0,1]$, which reads as

$$\int_0^1 f(x)\, \delta(x-a)\, dx = f(a), \;\; a \in (0,1)$$

to (5) we obtain the following formulas for approximations of eigenvalues:

$$\lambda_n^{(1)} = \left[u_n^{(0)}(a)\right]^2, \;\; \lambda_n^{(2)} = \left[u_n^{(0)}(a)\right]^2 I_0(a),$$

$$\lambda_n^{(3)} = \left[u_n^{(0)}(a)\right]^2 \left(-\left[u_n^{(0)}(a)\right]^2 I_1(a) + [I_0(a)]^2\right),$$

$$\lambda_n^{(4)} = \left[u_n^{(0)}(a)\right]^2 \left(\left[u_n^{(0)}(a)\right]^4 I_2(a) - 3\left[u_n^{(0)}(a)\right]^2 I_0(a)\, I_1(a) + [I_0(a)]^3\right),$$

$$\lambda_n^{(5)} = \left[u_n^{(0)}(a)\right]^2 \left(-\left[u_n^{(0)}(a)\right]^6 I_3(a) + \right.$$
$$+ \left[u_n^{(0)}(a)\right]^4 \left(4I_0(a)\, I_2(a) + 2\,[I_1(a)]^2\right) -$$
$$\left. - 6\left[u_n^{(0)}(a)\right]^2 [I_0(a)]^2\, I_1(a) + [I_0(a)]^4\right).$$

By setting $a = \dfrac{1}{\sqrt{2}}$ we obtain

$$I_0\left(\frac{1}{\sqrt{2}}\right) = \frac{\left(\sqrt{2}-1\right)\sin\left(\pi n\sqrt{2}\right)}{2n\pi} + \frac{\cos\left(\pi n\sqrt{2}\right) - 1}{4n^2\pi^2},$$

$$I_1\left(\frac{1}{\sqrt{2}}\right)=\frac{\left(3\sqrt{2}-4\right)\cos\left(\pi n\sqrt{2}\right)+1}{12n^2\pi^2}+$$
$$+\frac{\left(\sqrt{2}-1\right)\sin\left(\pi n\sqrt{2}\right)}{4n^3\pi^3}+\frac{3}{16}\frac{\cos\left(\pi n\sqrt{2}\right)-1}{n^4\pi^4},$$
$$I_2\left(\frac{1}{\sqrt{2}}\right)=-\frac{\left(2\sqrt{2}-3\right)\sin\left(\pi n\sqrt{2}\right)+1}{24n^3\pi^3}+\frac{\left(3\sqrt{2}-4\right)\cos\left(\pi n\sqrt{2}\right)+1}{16n^4\pi^4}+$$
$$+\frac{3\left(\sqrt{2}-1\right)\sin\left(\pi n\sqrt{2}\right)}{16n^5\pi^5}+\frac{5}{32}\frac{\cos\left(\pi n\sqrt{2}\right)-1}{n^6\pi^6},$$

$$I_3\left(\frac{1}{\sqrt{2}}\right)=-\frac{\left(30\sqrt{2}-43\right)\cos\left(\pi n\sqrt{2}\right)-2}{1440n^4\pi^4}-\frac{\left(2\sqrt{2}-3\right)\sin\left(\pi n\sqrt{2}\right)}{24n^5\pi^5}+$$
$$+\frac{5}{96}\frac{\left(3\sqrt{2}-4\right)\cos\left(\pi n\sqrt{2}\right)+1}{n^6\pi^6}+\frac{5}{32}\frac{\left(\sqrt{2}-1\right)\sin\left(\pi n\sqrt{2}\right)}{n^7\pi^7}+$$
$$+\frac{35}{256}\frac{\cos\left(\pi n\sqrt{2}\right)-1}{n^8\pi^8}.$$

From here we derive analytical expressions for the corrections to eigenvalues:

$$\lambda_n^{(1)}=1-\cos\left(\pi n\sqrt{2}\right),$$
$$\lambda_n^{(2)}=\frac{\sqrt{2}-1}{4n\pi}\left[2\sin\left(\pi n\sqrt{2}\right)-\sin\left(2\pi n\sqrt{2}\right)\right]+$$
$$+\frac{1}{8n^2\pi^2}\left[4\cos\left(\pi n\sqrt{2}\right)-\cos\left(2\pi n\sqrt{2}\right)-3\right],$$

$$\lambda_n^{(3)}=\frac{1}{48n^2\pi^2}\left[\left(27-15\sqrt{2}\right)\cos\left(\pi n\sqrt{2}\right)-\left(36-24\sqrt{2}\right)\cos\left(2\pi n\sqrt{2}\right)-\right.$$
$$\left.-\left(-13+9\sqrt{2}\right)\cos\left(3\pi n\sqrt{2}\right)-4\right]+$$
$$+\frac{\sqrt{2}-1}{8n^3\pi^3}\left[-5\sin\left(\pi n\sqrt{2}\right)+4\sin\left(2\pi n\sqrt{2}\right)-\sin\left(3\pi n\sqrt{2}\right)\right]-$$
$$-\frac{1}{16n^4\pi^4}\left[15\cos\left(\pi n\sqrt{2}\right)-6\cos\left(2\pi n\sqrt{2}\right)+\cos\left(3\pi n\sqrt{2}\right)-10\right],$$

$$\lambda_n^{(4)}=\frac{1}{96n^3\pi^3}\left[\left(33-26\sqrt{2}\right)\sin\left(\pi n\sqrt{2}\right)-\left(102-74\sqrt{2}\right)\sin\left(2\pi n\sqrt{2}\right)+\right.$$
$$\left.+\left(93-66\sqrt{2}\right)\sin\left(3\pi n\sqrt{2}\right)-\left(27-19\sqrt{2}\right)\sin\left(4\pi n\sqrt{2}\right)\right]+$$
$$+\frac{1}{128n^4\pi^4}\left[\left(84\sqrt{2}-160\right)\cos\left(\pi n\sqrt{2}\right)+\left(260-168\sqrt{2}\right)\cos\left(2\pi n\sqrt{2}\right)+\right.$$
$$\left.+\left(-160+108\sqrt{2}\right)\cos\left(3\pi n\sqrt{2}\right)+\left(35-24\sqrt{2}\right)\cos\left(4\pi n\sqrt{2}\right)+25\right]-$$

$$- \frac{3}{32n^5\pi^5}\left[-14\sin\left(\pi n\sqrt{2}\right)+14\sin\left(2\pi n\sqrt{2}\right)-6\sin\left(3\pi n\sqrt{2}\right)+\right.$$
$$\left.+\sin\left(4\pi n\sqrt{2}\right)\right]\left(\sqrt{2}-1\right)+\frac{5}{128n^6\pi^6}\left[56\cos\left(\pi n\sqrt{2}\right)-\right.$$
$$\left.-28\cos\left(2\pi n\sqrt{2}\right)+8\cos\left(3\pi n\sqrt{2}\right)-\cos\left(4\pi n\sqrt{2}\right)-35\right].$$

Symbolic and numerical computations were carried out using the computer algebra system Maple 17.00 (where `Digits=50`). The exact values of first four smallest eigenvalues are:

$$\lambda_1^{ex} \approx 11.02252382511,\ \ \lambda_2^{ex} \approx 41.34074086778,$$
$$\lambda_3^{ex} \approx 89.10712301833,\ \ \lambda_4^{ex} \approx 158.4324892201.$$

Numerical results are given in Table 1, where we show the absolute error of approximation to the eigenvalue $\left|\lambda_n^{ex} - \overset{m}{\lambda}_n\right|$, $n = \overline{1,4}$ calculated by the FD-method with the rank $m = \overline{1,7}$.

TABL. 1. Convergence of FD-method for the eigenvalues λ_n, $n = \overline{1,4}$.

m	$\left\lvert\lambda_1^{ex} - \overset{m}{\lambda}_1\right\rvert$	$\left\lvert\lambda_2^{ex} - \overset{m}{\lambda}_2\right\rvert$	$\left\lvert\lambda_3^{ex} - \overset{m}{\lambda}_3\right\rvert$	$\left\lvert\lambda_4^{ex} - \overset{m}{\lambda}_4\right\rvert$
0	1.1529194	1.8623232	$2.8068340 \cdot 10^{-1}$	$5.1881880 \cdot 10^{-1}$
1	$1.13335918 \cdot 10^{-1}$	$4.1070777 \cdot 10^{-3}$	$3.9480386 \cdot 10^{-3}$	$8.1111546 \cdot 10^{-3}$
2	$7.74223271 \cdot 10^{-3}$	$5.4659978 \cdot 10^{-3}$	$3.5908153 \cdot 10^{-5}$	$2.0458308 \cdot 10^{-5}$
3	$2.41326302 \cdot 10^{-4}$	$2.2361009 \cdot 10^{-4}$	$2.7688079 \cdot 10^{-6}$	$4.7899759 \cdot 10^{-6}$
4	$1.80327662 \cdot 10^{-5}$	$1.7567730 \cdot 10^{-5}$	$2.2495782 \cdot 10^{-8}$	$9.7346306 \cdot 10^{-8}$
5	$2.80813804 \cdot 10^{-6}$	$2.7903081 \cdot 10^{-6}$	$1.7826757 \cdot 10^{-9}$	$1.1955865 \cdot 10^{-9}$
6	$8.40809762 \cdot 10^{-8}$	$8.3989549 \cdot 10^{-8}$	$5.1188146 \cdot 10^{-11}$	$1.0727859 \cdot 10^{-10}$
7	$1.70181022 \cdot 10^{-8}$	$1.7004392 \cdot 10^{-8}$	$7.0536476 \cdot 10^{-13}$	$1.6910131 \cdot 10^{-12}$

One can see that the method converges for all eigenvalues including $n = 1$, even though condition (9) of theorem 2 is satisfied for $n \geq 2$ only.

3. General scheme of FD-method (for $\bar{q}(x) \not\equiv 0$)

If condition (9) is not valid, one has to apply the general FD-method technique. We intend to consider this case in the present section. For this purpose we embed problem (2) into the more general parametrical problem set

$$\begin{gathered}\frac{\partial^2 u(x,t)}{\partial x^2} + \left\{\lambda(t) - \sum_{p=1}^{k} \gamma_p \delta(x - x_p) - \hat{\psi}'(x) - \right.\\ \left. -t\left[\psi'(x) - \hat{\psi}'(x)\right]\right\} u(x,t) = 0,\\ x \in (0,1),\ u(0,t) = u(1,t) = 0,\end{gathered} \tag{18}$$

where $\psi(x)$ is the absolutely continuous function while $\hat{\psi}(x)$ stands for its piecewise linear approximation,

$$\hat{\psi}(x) = \psi(x_p)\frac{x_{p+1}-x}{x_{p+1}-x_p} + \psi(x_{p+1})\frac{x-x_p}{x_{p+1}-x_p},$$

$$\hat{\psi}'(x) = \psi_{x,p} = \frac{\psi(x_{p+1})-\psi(x_p)}{x_{p+1}-x_p},$$

$$x \in [x_p, x_{p+1}], \ \ p = \overline{0,k},$$

$$0 = x_0 < x_1 < ... < x_{k+1} = 1.$$

We look for the solution (18) in the form of series

$$u_n(x,t) = \sum_{j=0}^{\infty} u_n^{(j)}(x)\, t^j, \quad \lambda_n(t) = \sum_{j=0}^{\infty} \lambda_n^{(j)} t^j. \tag{19}$$

We substitute expressions (19) into (18) and then compare the coefficients in front of the equal powers of t. It gives us the following recurrence sequence of boundary problems:

$$\begin{cases} L_n^{(0)} u_n^{(j+1)}(x) \equiv \dfrac{d^2 u_n^{(j+1)}(x)}{dx^2} + \\ + \left\{ \lambda_n^{(0)} - \displaystyle\sum_{p=1}^{k} \gamma_p \delta(x-x_p) - \hat{\psi}'(x) \right\} u_n^{(j+1)}(x) = \\ = -\displaystyle\sum_{l=0}^{j} \lambda_n^{(j+1-l)} u_n^{(l)}(x) + \left[\psi'(x) - \hat{\psi}'(x)\right] u_n^{(j)}(x) \equiv \\ \equiv -F_n^{(j+1)}(x), \ x \in (0,1), \\ u_n^{(j+1)}(0) = u_n^{(j+1)}(1) = 0, \end{cases} \tag{20}$$

$$\lambda_n^{(j+1)} = \int_0^1 u_n^{(0)}(x) \left[\psi'(x) - \hat{\psi}'(x)\right] u_n^{(j)}(x)\, dx, \tag{21}$$

$$\int_0^1 u_n^{(0)}(x)\, u_n^{(j+1)}(x)\, dx = 0, \tag{22}$$

$$j = 0, 1, \dots .$$

Here the pair $\left\{\lambda_n^{(0)}, u_n^{(0)}(x)\right\} = \{\lambda_n(0), u_n(0)\}$ is the solution of the basic problem

$$\frac{\partial^2 u_n^{(0)}(x)}{\partial x^2} + \left\{ \lambda_n^{(0)} - \sum_{p=1}^{k} \gamma_p \delta(x-x_p) - \hat{\psi}'(x) \right\} u_n^{(0)}(x) = 0, \ x \in (0,1), \tag{23}$$
$$u_n^{(0)}(0) = u_n^{(0)}(1) = 0,$$

The sufficient conditions for the convergence of the series for $u_n(x,t)$ and $\lambda_n(t)$ at $t = 1$, where $u_n(x) = u_n(x,1)$, $\lambda_n = \lambda_n(1), n = 1, 2, ...,$ will be presented later. But first we give the algorithmic implementation of the FD-method.

Let us rewrite the problem (23) in the alternative form

$$\begin{gathered}\frac{\partial^2 u_n^{(0)}(x)}{\partial x^2}+\left\{\lambda_n^{(0)}-\hat{\psi}'(x)\right\}u_n^{(0)}(x)=0,\\ x\in(0,x_1)\cup(x_1,x_2)\cup\ldots\cup(x_k,1),\\ u_n^{(0)}(0)=u_n^{(0)}(1)=0,\end{gathered}\tag{24}$$

$$\left.\begin{aligned}&\left[u_n^{(0)}(x)\right]_{x=x_p}=u_n^{(0)}(x_p+0)-u_n^{(0)}(x_p-0)=0,\\ &\left[\frac{du_n^{(0)}(x)}{dx}\right]_{x=x_p}=\frac{du_n^{(0)}(x_p+0)}{dx}-\frac{du_n^{(0)}(x_p-0)}{dx}=\gamma_p u_n^{(0)}(x_p),\\ &\qquad p=\overline{1,k}.\qquad \text{(matching conditions)}\end{aligned}\right\}\tag{25}$$

On the intervals $[x_p,x_{p+1}),p=\overline{0,k-1}$ and $[x_k,1]$ the solutions of equation (24) can be written as follows

$$\begin{gathered}u_n^{(0)}(x)=A_{p,n}^{(0)}\sin\left(\sqrt{\mu_{n,p}^{(0)}}(x-x_p)\right)+\\ +B_{p,n}^{(0)}\cos\left(\sqrt{\mu_{n,p}^{(0)}}(x-x_p)\right),\quad x\in[x_p,x_{p+1}),\\ p=\overline{0,k-1},\qquad B_{0,n}^{(0)}=0,\\ u_n^{(0)}(x)=A_{k,n}^{(0)}\sin\left(\sqrt{\mu_{n,k}^{(0)}}(1-x)\right),x\in[x_k,1],\end{gathered}$$

where

$$\mu_{n,p}^{(0)}=\lambda_n^{(0)}-\psi_{x,p}.$$

The calculation of constants $A_{p,n}^{(0)}$, $p=\overline{0,k}$, $B_{p,n}^{(0)}$, $p=\overline{1,k-1}$ is performed using the combination of conditions (25) which when applied to the representation of solutions lead us to the following homogeneous system:

$$\begin{gathered}-A_{p-1,n}^{(0)}\sin\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p-x_{p-1})\right)-\\ -B_{p-1,n}^{(0)}\cos\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p-x_{p-1})\right)+B_{p,n}^{(0)}=0,\end{gathered}$$

$$\begin{gathered}-A_{p-1,n}^{(0)}\sqrt{\mu_{n,p-1}^{(0)}}\cos\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p-x_{p-1})\right)+\\ +B_{p-1,n}^{(0)}\sqrt{\mu_{n,p-1}^{(0)}}\sin\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p-x_{p-1})\right)+\\ +\sqrt{\mu_{n,p}^{(0)}}A_{p,n}^{(0)}-\gamma_p B_{p,n}^{(0)}=0,\quad p=\overline{1,k-1},\quad B_{0,n}^{(0)}=0,\end{gathered}\tag{26}$$

$$
\begin{gathered}
- A_{k-1,n}^{(0)} \sin\left(\sqrt{\mu_{n,k-1}^{(0)}}\left(x_k - x_{k-1}\right)\right) - \\
- B_{k-1,n}^{(0)} \cos\left(\sqrt{\mu_{n,k-1}^{(0)}}\left(x_k - x_{k-1}\right)\right) + \\
+ A_{k,n}^{(0)} \sin\left(\sqrt{\mu_{n,k}^{(0)}}\left(1 - x_k\right)\right) = 0, \\
- A_{k-1,n}^{(0)} \sqrt{\mu_{n,k-1}^{(0)}} \cos\left(\sqrt{\mu_{n,k-1}^{(0)}}\left(x_k - x_{k-1}\right)\right) + \\
+ B_{k-1,n}^{(0)} \sqrt{\mu_{n,k-1}^{(0)}} \sin\left(\sqrt{\mu_{n,k-1}^{(0)}}\left(x_k - x_{k-1}\right)\right) - \\
- A_{k,n}^{(0)} \left[\sqrt{\mu_{n,k}^{(0)}} \cos\left(\sqrt{\mu_{n,k}^{(0)}}\left(1 - x_k\right)\right) + \right. \\
\left. + \gamma_k \sin\left(\sqrt{\mu_{n,k}^{(0)}}\left(1 - x_k\right)\right)\right] = 0.
\end{gathered}
$$

We look for the roots of determinant $\Delta\left(\lambda_n^{(0)}\right)$ of system (26) which are different from $\psi_{x,p}$, $p = \overline{0,k}$. Every eigenvalue of problems (24)-(25) is the zero of determinant $\Delta\left(\lambda_n^{(0)}\right)$ having the multiplicity 1. The eigenvalues form a monotonically increasing sequence $\lambda_1^{(0)} < \lambda_2^{(0)} < ... < \lambda_n^{(0)} < ...$ which tends to infinity.

For the given $\lambda_n^{(0)}$ the solution to system (26) can be determined only up to a constant factor which we calculate from the normalization condition

$$
\left\|u_n^{(0)}\right\|_0 = \left\{\int_0^1 \left[u_n^{(0)}(x)\right]^2 dx\right\}^{\frac{1}{2}} = 1.
$$

The sequence of the normalized eigenfunctions $\left\{u_n^{(0)}(x)\right\}_{n=1}^{\infty}$ form a complete orthonormal system in $L_2[0,1]$. The above mentioned facts follow from the results of chapter 12 in [10].

Let us, move on to the solution of the recurrent sequence of problems (20)-(22). First we rewrite these equations in the equivalent form

$$
\begin{gathered}
\hat{L}_n^{(0)} u_n^{(j+1)}(x) \equiv \frac{d^2 u_n^{(j+1)}(x)}{dx^2} + \mu_n^{(0)} u_n^{(j+1)}(x) = -F_n^{(j+1)}(x), \\
x \in (0, x_1) \cup (x_1, x_2) \cup ... \cup (x_k, 1), \\
\mu_n^{(0)}(x) = \mu_{n,p}^{(0)}, \ x \in (x_p, x_{p+1}), \ p = \overline{0,k}, \\
u_n^{(j+1)}(0) = u_n^{(j+1)}(1) = 0,
\end{gathered} \tag{27}
$$

$$
\left.
\begin{aligned}
&\left[u_n^{(j+1)}(x)\right]_{x=x_p} = 0, \\
&\left[\frac{du_n^{(j+1)}(x)}{dx}\right]_{x=x_p} = \gamma_p u_n^{(j+1)}(x_p), p = \overline{1,k}.
\end{aligned}
\right\} \text{(matching conditions)}
$$

Whereupon, its solution possess a representation

$$u_n^{(j+1)}(x) = A_{p,n}^{(j+1)} \sin\left(\sqrt{\mu_{n,p}^{(0)}}(x - x_p)\right) + B_{p,n}^{(j+1)} \cos\left(\sqrt{\mu_{n,p}^{(0)}}(x - x_p)\right) - \int_{x_p}^{x} \frac{\sin\left(\sqrt{\mu_{n,p}^{(0)}}(x - \xi)\right)}{\sqrt{\mu_{n,p}^{(0)}}} F_n^{(j+1)}(\xi)\, d\xi,\ x \in [x_p, x_{p+1}),$$

$$p = \overline{0, k-1}, \quad B_{0,n}^{(j+1)} = 0,$$

$$u_n^{(j+1)}(x) = A_{k,n}^{(j+1)} \sin\left(\sqrt{\mu_{n,k}^{(0)}}(1 - x)\right) + \int_{x}^{1} \frac{\sin\left(\sqrt{\mu_{n,k}^{(0)}}(x - \xi)\right)}{\sqrt{\mu_{n,k}^{(0)}}} F_n^{(j+1)}(\xi)\, d\xi, \quad x \in [x_k, 1].$$

By combining (27) and the matching conditions we obtain the following system for coefficients $A_{p,n}^{(j+1)}$, $B_{p,n}^{(j+1)}$:

$$\begin{gathered}
-A_{p-1,n}^{(j+1)} \sin\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p - x_{p-1})\right) - B_{p-1,n}^{(j+1)} \cos\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p - x_{p-1})\right) + \\
+ B_{p,n}^{(j+1)} = -\int_{x_{p-1}}^{x_p} \frac{\sin\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p - \xi)\right)}{\sqrt{\mu_{n,p-1}^{(0)}}} F_n^{(j+1)}(\xi)\, d\xi, \\
-A_{p-1,n}^{(j+1)} \sqrt{\mu_{n,p-1}^{(0)}} \cos\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p - x_{p-1})\right) + B_{p-1,n}^{(j+1)} \sqrt{\mu_{n,p-1}^{(0)}} \times \\
\times \sin\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p - x_{p-1})\right) + \sqrt{\mu_{n,p}^{(0)}} A_{p,n}^{(j+1)} - \gamma_p B_{p,n}^{(j+1)} = \\
= -\int_{x_{p-1}}^{x_p} \cos\left(\sqrt{\mu_{n,p-1}^{(0)}}(x_p - \xi)\right) F_n^{(j+1)}(\xi)\, d\xi, \\
p = \overline{1, k-1}, \qquad B_{0,n}^{(j+1)} = 0, \\
-A_{k-1,n}^{(j+1)} \sin\left(\sqrt{\mu_{n,k-1}^{(0)}}(x_k - x_{k-1})\right) - \\
- B_{k-1,n}^{(j+1)} \cos\left(\sqrt{\mu_{n,k-1}^{(0)}}(x_k - x_{k-1})\right) + \\
+ A_{k,n}^{(j+1)} \sin\left(\sqrt{\mu_{n,k}^{(0)}}(1 - x_k)\right) =
\end{gathered} \tag{28}$$

$$= -\int_{x_k}^{1} \frac{\sin\left(\sqrt{\mu_{n,k}^{(0)}}\,(x_k-\xi)\right)}{\sqrt{\mu_{n,k}^{(0)}}} F_n^{(j+1)}(\xi)\,d\xi -$$
$$- \int_{x_{k-1}}^{x_k} \frac{\sin\left(\sqrt{\mu_{n,k-1}^{(0)}}\,(x_k-\xi)\right)}{\sqrt{\mu_{n,k-1}^{(0)}}} F_n^{(j+1)}(\xi)\,d\xi,$$
$$- A_{k-1,n}^{(j+1)}\sqrt{\mu_{n,k-1}^{(0)}}\cos\left(\sqrt{\mu_{n,k-1}^{(0)}}\,(x_k-x_{k-1})\right) +$$
$$+ B_{k-1,n}^{(j+1)}\sqrt{\mu_{n,k-1}^{(0)}}\sin\left(\sqrt{\mu_{n,k-1}^{(0)}}\,(x_k-x_{k-1})\right) -$$
$$- A_{k,n}^{(j+1)}\left[\sqrt{\mu_{n,k}^{(0)}}\cos\left(\sqrt{\mu_{n,k}^{(0)}}\,(1-x_k)\right) +\right.$$
$$\left.+\gamma_k \sin\left(\sqrt{\mu_{n,k}^{(0)}}\,(1-x_k)\right)\right] = -\int_{x_k}^{1} \cos\left(\sqrt{\mu_{n,k}^{(0)}}\,(x_k-\xi)\right) F_n^{(j+1)}(\xi)\,d\xi -$$
$$- \int_{x_{k-1}}^{x_k} \cos\left(\sqrt{\mu_{n,k-1}^{(0)}}\,(x_k-\xi)\right) F_n^{(j+1)}(\xi)\,d\xi +$$
$$+ \gamma_k \int_{x_k}^{1} \frac{\sin\left(\sqrt{\mu_{n,k}^{(0)}}\,(x_k-\xi)\right)}{\sqrt{\mu_{n,k}^{(0)}}} F_n^{(j+1)}(\xi)d\xi.$$

The left-hand-side matrix of this system of linear algebraic equations is degenerate since it coincides with that of the system (26). For the solution of (28) to exist it is necessary and sufficient that the vector composed from the right-hand-side coefficients is orthogonal to the eigenvector of the conjugate matrix.

Let us introduce the following vectors

$$\vec{Y}_n^{(j+1)} = \left\{ A_{0,n}^{(j+1)}, \underbrace{A_{1,n}^{(j+1)}, B_{1,n}^{(j+1)}}, \ldots, \underbrace{A_{k-1,n}^{(j+1)}, B_{k-1,n}^{(j+1)}}, A_{k,n}^{(j+1)} \right\}^T,$$
$$\vec{H}_n^{(j+1)} = \left\{ \vec{H}_{n,p}^{(j+1)} \right\}_{p=\overline{1,k}}^T,$$
$$\vec{H}_{n,p}^{(j+1)} = \left\{ -\int_{x_{p-1}}^{x_p} \frac{\sin\left(\sqrt{\mu_{n,p-1}^{(0)}}\,(x_p-\xi)\right)}{\sqrt{\mu_{n,p-1}^{(0)}}} F_n^{(j+1)}(\xi)\,d\xi,\right.$$
$$\left. - \int_{x_{p-1}}^{x_p} \cos\left(\sqrt{\mu_{n,p-1}^{(0)}}\,(x_p-\xi)\right) F_n^{(j+1)}(\xi)\,d\xi \right\},$$

$$p = \overline{1, k-1},$$

$$\vec{H}_{n,k}^{(j+1)} = \left\{ -\int_{x_k}^{1} \frac{\sin\left(\sqrt{\mu_{n,k}^{(0)}}\,(x_k-\xi)\right)}{\sqrt{\mu_{n,k}^{(0)}}} F_n^{(j+1)}(\xi)\,d\xi - \right.$$

$$- \int_{x_{k-1}}^{x_k} \frac{\sin\left(\sqrt{\mu_{n,k-1}^{(0)}}\,(x_k-\xi)\right)}{\sqrt{\mu_{n,k-1}^{(0)}}} F_n^{(j+1)}(\xi)\,d\xi,$$

$$- \int_{x_k}^{1} \cos\left(\sqrt{\mu_{n,k}^{(0)}}\,(x_k-\xi)\right) F_n^{(j+1)}(\xi)\,d\xi -$$

$$- \int_{x_{k-1}}^{x_k} \cos\left(\sqrt{\mu_{n,k-1}^{(0)}}\,(x_k-\xi)\right) F_n^{(j+1)}(\xi)\,d\xi +$$

$$\left. + \gamma_k \int_{x_k}^{1} \frac{\sin\left(\sqrt{\mu_{n,k}^{(0)}}\,(x_k-\xi)\right)}{\sqrt{\mu_{n,k}^{(0)}}} F_n^{(j+1)}(\xi)\,d\xi \right\}$$

and denote the matrix of the system (26) as D_n. Then systems (26), (28) could be presented in the matrix-vector form

$$D_n \vec{Y}_n^{(0)} = \vec{0}, \;\; D_n \vec{Y}_n^{(j+1)} = \vec{H}_n^{(j+1)}, \;\; j = 0, 1, \ldots . \tag{29}$$

If $\vec{Z}_n^T$ is the eigenvector (row) that corresponds to the null eigenvalue of the matrix D_n, i.e.

$$\vec{Z}_n^T D_n = \vec{0},$$

then the necessary and sufficient condition of the solvability of system (29) is

$$\vec{Z}_n^T \vec{H}_n^{(j+1)} = 0. \tag{30}$$

It is easy to show that condition (30) is equivalent to the integral condition having the form

$$\int_0^1 F_n^{(j+1)}(x)\, u_n^{(0)}(x)\,dx = 0. \tag{31}$$

Next we wind from (31) or, equivalently, from (30) that

$$\lambda_n^{(j+1)} = -\sum_{p=1}^{j} \lambda_n^{(j-p+1)} \int_0^1 u_n^{(0)}(x)\, u_n^{(p)}(x)\,dx + \\ + \int_0^1 u_n^{(0)}(x) \left[\psi'(x) - \hat{\psi}'(x)\right] u_n^{(j)}(x)\,dx. \tag{32}$$

Since the solution of system of linear algebraic equations (29) is found with the accuracy up to a constant factor, $u_n^{(j+1)}(x)$ is found with the same accuracy.

The constant factor can be calculated from the orthogonality condition (22), and formula (32) is transformed to (21).

The aforementioned results give us all information necessary to apply FD-method to some concrete problem. They however are not so useful to get the sufficient conditions of its convergence and the corresponding accuracy estimates (both a-priory and a-posteriori).

To get those estimates we propose an alternative approach. Relying on the completeness of the orthonormalized system $\left\{u_n^{(0)}(x)\right\}_{n=1}^{\infty}$ in $L_2[0,1]$, we write down the solution to problem (20) in the following form:

$$u_n^{(j+1)}(x) = -\sum_{\substack{p=1\\p\neq n}}^{\infty} \int_0^1 F_n^{(j+1)}(\xi)\, u_p^{(0)}(\xi)\, d\xi \frac{u_p^{(0)}(x)}{\lambda_n^{(0)} - \lambda_p^{(0)}}.$$

It lead us to the estimate

$$\begin{aligned} \left\|u_n^{(j+1)}\right\| &\le M_n \left\|F_n^{(j+1)}\right\| \le \\ &\le M_n \left\{ \sum_{l=1}^{j} \left|\lambda_n^{(j+1-l)}\right| \left\|u_n^{(l)}\right\| + \left\| \left[\psi'(x) - \hat{\psi}'(x)\right] u_n^{(j)}(x) \right\| \right\}, \end{aligned} \tag{33}$$

where

$$M_n = \max\left\{ \frac{1}{\lambda_n^{(0)} - \lambda_{n-1}^{(0)}}, \frac{1}{\lambda_{n+1}^{(0)} - \lambda_n^{(0)}} \right\}. \tag{34}$$

Let us introduce a function

$$\omega(\psi') = \max_{0\le p\le k} \max_{x\in[x_p, x_{p+1}]} \left| \int_{x_p}^{x_{p+1}} \frac{\psi'(x) - \psi'(t)}{x_{p+1} - x_p} dt \right|.$$

Then by substituting (21) into (33) we receive the sequence of estimates

$$\begin{aligned} &\left\|u_n^{(j+1)}\right\| \le M_n \left\{ \sum_{l=1}^{j} \left|\lambda_n^{(j+1-l)}\right| \left\|u_n^{(l)}\right\| + \omega(\psi') \left\|u_n^{(j)}\right\| \right\}, \\ &\left|\lambda_n^{(j+1)}\right| \le \omega(\psi') \left\|u_n^{(j)}\right\|, \end{aligned} \tag{35}$$

that lead to the following inequality

$$\left\|u_n^{(j+1)}\right\| \le M_n \omega(\psi') \sum_{l=0}^{j} \left\|u_n^{(j-l)}\right\| \left\|u_n^{(l)}\right\|. \tag{36}$$

The solution of inequality (36) be obtained via the generating functions method. It has a following form (see [24])

$$\begin{aligned} \left\|u_n^{(j+1)}\right\| &\le \left(4M_n\omega(\psi')\right)^{j+1} 2\frac{(2j+1)!!}{(2j+4)!!} \le \\ &\le \frac{\left[4M_n\omega(\psi')\right]^{j+1}}{(j+2)\sqrt{\pi(j+1)}} = \frac{\hat{r}_n^{j+1}}{(j+2)\sqrt{\pi(j+1)}}. \end{aligned} \tag{37}$$

Inequality (37) permit us to get the corresponding inequality for the eigenvalue from (35)

$$\left|\lambda_n^{(j+1)}\right| \le \omega\left(\psi'\right)\hat{r}_n^j\, 2\frac{(2j-1)!!}{(2j+2)!!} \le \omega\left(\psi'\right)\frac{\hat{r}_n^j}{(j+1)\sqrt{\pi j}}. \tag{38}$$

Using estimates (37), (38) one can easily deduce that the next statement is correct

Theorem 3. *Let*

$$\sigma(x) = \sum_{p=1}^{k}\gamma_p H(x - x_p) + \psi(x) \tag{39}$$

and the following condition holds true

$$\hat{r}_n \stackrel{def}{=} 4M_n\omega\left(\psi'\right) < 1,$$

then the FD-method for the Sturm–Liouville problem (18), (39) converges super-exponentially. Moreover the following error estimates are valid:

$$\left\|u_n - \overset{m}{u}_n\right\| \le \left\|u_n - \sum_{j=0}^{m}u_n^{(j)}\right\| \le \frac{\hat{r}_n^{m+1}}{(m+2)\sqrt{\pi(m+1)}\,(1-\hat{r}_n)}, \tag{40}$$

$$\left|\lambda_n - \overset{m}{\lambda}_n\right| \le \left|\lambda_n - \sum_{j=0}^{m}\lambda_n^{(j)}\right| \le \frac{\omega\left(\psi'\right)\hat{r}_n^m}{(m+1)\sqrt{\pi m}\,(1-\hat{r}_n)}. \tag{41}$$

Remark 3.1. *In order to to understand the behavior of $\hat{r}_n$ with respect to n one can use (34) and theorem 2. They lead to the estimates on the denominator from* (34)

$$\begin{aligned}\lambda_n^{(0)} - \lambda_{n-1}^{(0)} &= \pi^2(2n-1) + \\ &+ 2\sum_{p=1}^{k}\gamma_p\left[\sin^2(n\pi x_p) - \sin^2((n-1)\pi x_p)\right] + R_n^{(2)} - R_{n-1}^{(2)} \ge \\ &\ge \pi^2(2n-1) - 4\sum_{p=1}^{k}|\gamma_p| - \frac{2\sum_{p=1}^{k}|\gamma_p|}{2\sqrt{\pi}}\left[\frac{\hat{r}_n}{1-\hat{r}_n} + \frac{\hat{r}_{n-1}}{1-\hat{r}_{n-1}}\right],\end{aligned}$$

$$\lambda_{n+1}^{(0)} - \lambda_n^{(0)} \ge \pi^2(2n+1) - 4\sum_{p=1}^{k}|\gamma_p| - \frac{\sum_{p=1}^{k}|\gamma_p|}{\sqrt{\pi}}\left[\frac{\hat{r}_{n+1}}{1-\hat{r}_{n+1}} + \frac{\hat{r}_n}{1-\hat{r}_n}\right],$$

These estimates are valid under condition (9), i.e. estimates (40), (41) and (10), (11) from the theorem 2 are valid under the same restriction on n. However, $\hat{r}_n$ has a reserve of easing the restrictions on n up to its complete exclusion. This reserve caused by the occurrence of factor $\omega(\psi')$ in $\hat{r}_n$ that will relax the restrictions on n provided that function $\psi'(x)$ is, at least, piecewise continuous function from $Q^0[0,1]$, i.e. $\psi(x) \in C[0,1] \cap Q^1[0,1]$.

Remark 3.2. *If the conditions of theorem 3 are met then the series $u_n(x,t) = \sum_{j=0}^{\infty}u_n^{(j)}(x)t^j$, $\lambda_n(t) = \sum_{j=0}^{\infty}\lambda_n^{(j)}t^j$ are absolutely convergent* *for* $|t| \leq 1$. *Moreover they approximate the exact solution of given problem* $u_n(x) = u_n(x,1) = \sum_{j=0}^{\infty} u_n^{(j)}(x)$, $\lambda_n = \lambda_n(1) = \sum_{j=0}^{\infty} \lambda_n^{(j)}$.

Example 3.1. We applied the FD-method to problem (2) with the potential $q(x) = \delta\left(x - \frac{1}{2}\right) + 100x$ in the following cases: a) $\hat{\psi}'(x) \equiv 0$, $k = 1$, $x_1 = \frac{1}{2}$, $\gamma_1 = 1$; b) the interval $(0,1)$ is partitioned into two equal subintervals ($\hat{\psi}'(x) \not\equiv 0$, $k = 1$, $x_1 = \frac{1}{2}$,$\gamma_1 = 1$); c) the interval $(0,1)$ is partitioned into four equal subintervals ($\hat{\psi}'(x) \not\equiv 0$, $k = 3$, $x_1 = \frac{1}{4}, x_2 = \frac{1}{2}, x_3 = \frac{3}{4}$, $\gamma_1 = 0$, $\gamma_2 = 1$, $\gamma_3 = 0$).

TABL. 2. Convergence of FD-method for eigenvalue λ_1

m	a) $\hat{\psi}'(x) \equiv 0$, $k = 1$, $\left\lvert\lambda_1^{ex} - \overset{m}{\lambda}_1\right\rvert$	b) $\hat{\psi}'(x) \not\equiv 0$, $k = 1$, $\left\lvert\lambda_1^{ex} - \overset{m}{\lambda}_1\right\rvert$	c) $\hat{\psi}'(x) \not\equiv 0$, $k = 3$, $\left\lvert\lambda_1^{ex} - \overset{m}{\lambda}_1\right\rvert$
0	39.79669103	2.270616222	$2.168801379 \cdot 10^{-1}$
1	10.20330897	$8.341737964 \cdot 10^{-1}$	$6.083140294 \cdot 10^{-2}$
2	2.135818380	$1.901098870 \cdot 10^{-2}$	$5.300909434 \cdot 10^{-5}$
3	2.135818380	$3.157060409 \cdot 10^{-3}$	$4.333553271 \cdot 10^{-6}$
4	1.226920389	$2.930165507 \cdot 10^{-4}$	$1.367746278 \cdot 10^{-8}$
5	1.226920389	$2.102813177 \cdot 10^{-5}$	$5.850330410 \cdot 10^{-10}$
6	$9.509541771 \cdot 10^{-1}$	$4.743628885 \cdot 10^{-6}$	$3.835005760 \cdot 10^{-12}$
7	$9.509541771 \cdot 10^{-1}$	$5.240882809 \cdot 10^{-8}$	$9.702842701 \cdot 10^{-14}$
8	$8.506978298 \cdot 10^{-1}$	$7.286716281 \cdot 10^{-8}$	$1.229092383 \cdot 10^{-15}$
9	$8.506978298 \cdot 10^{-1}$	$2.930256199 \cdot 10^{-9}$	$1.865391361 \cdot 10^{-17}$
10	$8.276761403 \cdot 10^{-1}$	$1.032042190 \cdot 10^{-9}$	$4.064792983 \cdot 10^{-19}$
11	$8.276761403 \cdot 10^{-1}$	$1.038538699 \cdot 10^{-10}$	$3.423104476 \cdot 10^{-21}$
12	$8.508842593 \cdot 10^{-1}$	$1.221151730 \cdot 10^{-11}$	$1.238050539 \cdot 10^{-22}$
13	$8.508842593 \cdot 10^{-1}$	$2.481662360 \cdot 10^{-12}$	$3.497226425 \cdot 10^{-25}$
14	$9.094304891 \cdot 10^{-1}$	$8.479672332 \cdot 10^{-14}$	$3.323469489 \cdot 10^{-26}$
15	$9.094304891 \cdot 10^{-1}$	$4.980766446 \cdot 10^{-14}$	$1.068874105 \cdot 10^{-28}$
16	1.000506593	$1.155397490 \cdot 10^{-15}$	$7.886548397 \cdot 10^{-30}$
17	1.000506593	$8.676674901 \cdot 10^{-16}$	$9.000481917 \cdot 10^{-32}$
18	1.125540512	$6.964067548 \cdot 10^{-17}$	$1.660871600 \cdot 10^{-33}$
19	1.125540512	$1.270480995 \cdot 10^{-17}$	$4.098653028 \cdot 10^{-35}$
20	1.288866993	$2.045466355 \cdot 10^{-18}$	$2.760733186 \cdot 10^{-37}$

We computed the exact eigenvalue (further denoted by λ_1^{ex}) and its approximation (denoted by λ_1) using the computer algebra system Maple 17.00 (`Digits=100`). The smallest exact eigenvalue of the problem, considered here, is equal to

$$\lambda_1^{ex} \approx 51.5685501948004855889197393511906843908 5.$$

The absolute errors of approximations $\left\lvert\lambda_1^{ex} - \overset{m}{\lambda}_1\right\rvert$ to smallest eigenvalue λ_1 obtained using the FD-method of rank $m = \overline{1, 20}$ in the cases a)-c) are presented in table 2.

One can see from the table 2 that the simplest form of the FD-method a) (with $\hat{\psi}'(x) \equiv 0$) for the first eigenvalue is divergent while the FD-method converges when the interval is partitioned into two or more subintervals. The convergence rate is doubled with increase in the number of subdivision points (from one to three).

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