Representation of solutions to the one-dimensional Schrödinger equation in terms of Neumann series of Bessel functions

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Abstract

A new representation of solutions to the equation $-y'' + q(x)y = \omega^2 y$ is obtained. For every $x$ the solution is represented as a Neumann series of Bessel functions depending on the spectral parameter $\omega$. Due to the fact that the representation is obtained using the corresponding transmutation operator, a partial sum of the series approximates the solution uniformly with respect to $\omega$ which makes it especially convenient for the approximate solution of spectral problems. The numerical method based on the proposed approach allows one to compute large sets of eigendata with a non-deteriorating accuracy.

1 Introduction

We consider the equation

\begin{equation}
- y'' + q(x)y = \omega^2 y
\end{equation}

on a finite interval $(0, b)$. We assume $q$ being a continuous complex valued function of an independent real variable $x \in [0, b]$ and $\omega$ an arbitrary complex number.

The main result of the paper is a new representation for solutions of (1.1) and for their derivatives in the form of Neumann series of Bessel functions with explicit formulas for the coefficients. We obtain that two linearly independent solutions of (1.1) have the form

\begin{equation}
c(\omega, x) = \cos \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n}(x) j_{2n}(\omega x)
\end{equation}

and

\begin{equation}
s(\omega, x) = \sin \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n+1}(x) j_{2n+1}(\omega x)
\end{equation}

where $j_k$ stands for the spherical Bessel function of order $k$ and the functions $\beta_k$ are calculated following a relatively simple recursive integration procedure. The series are uniformly convergent both with respect to $x$ and to $\omega$. The representations are obtained with the aid of the transmutation (transformation) operators related with (1.1) (for the theory of such operators we refer to \[4\], \[9\], \[33\], \[35\], \[41\], \[45\]). Due to this fact and since the kernel of a transmutation operator, realized in the form of a Volterra integral operator, is independent of the spectral parameter, it is not difficult to prove that the partial sums of the series obtained

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approximate the solutions uniformly with respect to $\omega$ (Theorem 4.1 and Remark 5.3). This makes them especially attractive for approximate solving of spectral problems.

The possibility to dispose of explicit formulas (3.1) for the coefficients $\beta_k$ in the series comes from a mapping property of the transmutation operators discovered in [8], see also [29] and [30]. Due to that property, in spite of not knowing the kernel of the transmutation operator, one can however construct the set of images under the action of the transmutation operator of all nonnegative integer powers of the independent variable $x$. Using this we obtain a Fourier-Legendre expansion of the transmutation kernel and use it to write down the new representations for solutions of (1.1). Estimates for the rate of convergence of the Fourier-Legendre series are obtained in dependence on the smoothness of $q$.

The efficiency and the uniform accuracy of the solution representations is illustrated by some numerical examples which show that in several seconds one can compute hundreds or if necessary thousands of eigendata with essentially the same and small enough absolute error.

The one-dimensional Schrödinger equation (1.1) is, of course, one of the most fundamental and classical objects of study in the theory of differential equations and mathematical physics. Its applications are uncountable. Any new result for this equation and especially a new representation of its solutions can lead to unforeseen applications. Since the new representation possesses such a unique and, in fact, amazing feature of uniformity with respect to the spectral parameter $\omega$, its clear and immediate application is to approximate solution of spectral and scattering problems. We explore this use of our main result and show that without using any elaborate numerical technique and simply programming the analytical formulas obtained in the present work one can compute huge amounts of eigendata with a uniform accuracy guaranteed, very fast, and in general for complex valued coefficients. At present no other algorithm offers similar possibilities, and we emphasize that a new numerical method is only one possible application of the representation obtained. We expect that the new representation will be used for obtaining asymptotic relations and solving inverse problems. Moreover, a crucial role is played by the transmutation operator. This is another fundamental object of the theory of differential equations and especially of the theory of inverse spectral and scattering problems. Its basic properties are well understood, but the difficulties with construction of its integral kernel have always restricted its practical use. In this relation we mention the paper [6] where analytic approximation formulas for the integral kernel were obtained and the recent publications [29], [30] where another procedure of analytical approximation was proposed. To the difference of those previous results, in the present work we obtain an exact formula for the transmutation operator, its kernel is represented in the form of a Fourier-Legendre series with explicit formulas for the coefficients. The use of the transmutation operator is not limited to Sturm-Liouville equations. In particular, it is applied to relate partial differential equations (see, e.g., [4]) and hence to solve problems involving PDEs with variable coefficients. The representation of the transmutation kernel proposed here has a convenient structure for this sort of applications. For example, it may be used to construct complete systems of solutions of PDEs related via the transmutation to those with known complete systems of solutions (see, e.g., [12]).

Finally, let us notice that the Neumann series of Bessel functions represent another classical notion of mathematical analysis. They were first studied by the German mathematician Carl Gottfried Neumann in 1867 and are named after him. The theory of Neumann series was developed later by L. B. Gegenbauer in 1877. We refer to another important paper on this subject [15]. For more recent results we refer to [2], [37] and references therein. In an interesting research reported in [11] and [10] there appears a representation of solutions of Sturm-Liouville equations in the form of Neumann series of Bessel functions different to the representation obtained in the present work. The representation from [11] and [16] does not possess the uniformity with respect to $\omega$ to the difference from our representation, and the convergence of the series which is guaranteed on a certain interval of $x$ for holomorphic $q$ only is achieved due to the exponential decay of $j_n(z)$ when $n \to \infty$. Apart from that previous work, to our best knowledge, the Neumann series of Bessel functions have not been used to represent solutions of a general linear differential equation. The attractive features of the representation presented here indicate that the Neumann series of Bessel functions should be considered as a natural and important object of study in the theory of linear differential equations.

The paper is structured as follows. In Section 2 we introduce some necessary notations, definitions and properties concerning special systems of functions related to (1.1) and called formal powers, as well as the transmutation operators. In Section 3 we show that the kernel of a transmutation operator admits the representation $K(x,t) = \sum_{k=0}^{\infty} \frac{\beta_k(x)}{x} P_k \left( \frac{t}{x} \right)$ where $P_k$ are Legendre polynomials and the coefficients $\beta_k$ are defined with the aid of the formal powers. We prove a direct and an inverse results on the rate of
convergence of the series in dependence on the smoothness of \( q \). In Section 4 the Fourier-Legendre expansion of the transmutation kernel is used to obtain the main result of this work, the representations (1.2) and (1.3), and to prove that the partial sums of these series give us a uniform approximation of the solutions with respect to the spectral parameter \( \omega \). In Section 5 we obtain analogous results for the derivatives of the solutions \( c(\omega, x) \) and \( s(\omega, x) \). Again we prove the uniform approximation with respect to \( \omega \). Since the coefficients \( \beta_k \) (and their counterparts \( \gamma_k \) appearing in the representations of the derivatives) are the main ingredient of the representations which depends on \( q \), besides their direct definition in terms of formal powers (3.1) it is desirable to dispose of a most efficient and stable procedure for their numerical computation. In Section 6 we propose one such procedure which proved to work numerically much better than (3.1) and converted the representations (1.2) and (1.3) into a powerful numerical method for solving initial value and spectral problems for (1.1). In Section 7 we confirm this affirmation with several numerical experiments.

2 Transmutations and formal powers

The definition of the transmutation operator as given in this paper requires the potential \( q \) to be defined on the symmetric interval \([-b, b]\) (see [35], [29]). However as we explain later in this section, the results of the present work do not depend on the continuation of the potential onto negative values of \( x \). For that reason throughout this section we assume that equation (1.1) is defined on the symmetric segment \([-b, b]\) and that the potential \( q \) is continuous on this segment and in the rest of the paper only the segment \([0, b]\) is considered.

Throughout the paper we suppose that \( f \) is a non-vanishing solution (in general, complex-valued) of the equation

\[
f'' - qf = 0
\]

on \([0, b]\) (\([-b, b]\) for this section) such that

\[f(0) = 1.\]

The existence of such solution for any complex-valued \( q \in C[-b, b] \) was proved in [26, Remark 5] (see also [7]). Denote \( h := f'(0) \).

Consider two sequences of recursive integrals (see [23], [25], [26])

\[
X^{(0)}(x) \equiv 1, \quad X^{(n)}(x) = n \int_0^x X^{(n-1)}(s) \left(f^2(s)\right)^{\frac{-1}{n}} \, ds, \quad n = 1, 2, \ldots
\]

and

\[
\tilde{X}^{(0)}(x) \equiv 1, \quad \tilde{X}^{(n)}(x) = n \int_0^x \tilde{X}^{(n-1)}(s) \left(f^2(s)\right)^{\frac{-1}{n-1}} \, ds, \quad n = 1, 2, \ldots.
\]

**Definition 2.1.** The families of functions \( \{\varphi_k\}_{k=0}^{\infty} \) and \( \{\psi_k\}_{k=0}^{\infty} \) constructed according to the rules

\[
\varphi_k(x) = \begin{cases} f(x)X^{(k)}(x), & k \text{ odd}, \\ f(x)\tilde{X}^{(k)}(x), & k \text{ even} \end{cases}
\]

and

\[
\psi_k(x) = \begin{cases} \tilde{X}^{(k)}(x), & k \text{ odd}, \\ f(x)\tilde{X}^{(k)}(x), & k \text{ even}. \end{cases}
\]

are called the systems of formal powers associated with \( f \).

**Remark 2.2.** The formal powers arise in the spectral parameter power series (SPPS) representation for solutions of (1.1) (see [21], [23], [25], [26]).

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\[1\] In fact the only reason for the requirement of the absence of zeros of the function \( f \) is to make sure that the auxiliary functions \( \varphi_k \) and \( \psi_k \) be well defined. As was shown in [25] this can be done even without such requirement, but corresponding formulas are relatively more complicated.
Theorem 2.3. Let \( q \in C[-b, b] \). Then there exists a unique complex valued function \( K(x, t) \in C^1([-b, b] \times [-b, b]) \) such that the Volterra integral operator

\[
T u(x) = u(x) + \int_{-x}^{x} K(x, t) u(t) dt
\]

defined on \( C[-b, b] \) satisfies the equality

\[
\left( -\frac{d^2}{dx^2} + q(x) \right) T[u] = T \left[ -\frac{d^2}{dx^2}(u) \right]
\]

for any \( u \in C^2[-b, b] \) and

\[
T[1] = f.
\]

For the proof of this fact we refer to [84, Theorem 3.1.1]. Slightly different proof and references to earlier publications are given in [29].

\( T \) maps any solution \( v \) of the equation \( v'' + \omega^2 v = 0 \) into a solution \( y \) of equation (1.1) with the following correspondence of the initial values \( y(0) = v(0), y'(0) = v'(0) + hv(0) \).

In particular, we introduce two linearly independent solutions of (1.1),

\[
c(\omega, x) := T[\cos \omega x] \quad \text{and} \quad s(\omega, x) := T[\sin \omega x].
\]

Note that the definition of the transmutation operator (2.4) requires knowledge of the integral kernel \( K \) only in the regions \( R_1 := \{ 0 \leq x \leq b, |t| \leq x \} \) and \( R_2 := \{-b \leq x \leq 0, |t| \leq |x| \} \). Moreover, these two regions are independent in the following sense. The integral kernel \( K \) in \( R_1 \) depends on the values of the potential \( q \) only on \([0, b]\) and does not depend on values for \( x < 0 \) (see (2.5)), and in \( R_2 \) depends on the values on \([-b, 0]\) and does not depend on the values for \( x > 0 \). The value of \( T[u](x) \) for \( x \geq 0 \) does not require the knowledge of \( K \) on \( R_2 \). The same happens to the formal powers \( \{ \varphi_k \} \) and \( \{ \psi_k \} \) whose values on \([0, b]\) are independent on the potential \( q \) on \([-b, 0]\). Therefore from now on we restrict the presentation to the segment \([0, b]\), all the results for the segment \([-b, 0]\) are similar. One of the advantages of restricting the consideration to the segment \([0, b]\) consists in the knowledge of the initial values of the solutions \( c(\omega, x) \) and \( s(\omega, x) \) in the origin which is convenient for solving initial value and spectral problems on \([0, b]\).

The following mapping property plays a crucial role in what follows.

Proposition 2.4 (8).

\[
T \left[ x^k \right] = \varphi_k(x) \quad \text{for any } k \in \mathbb{N} \cup \{ 0 \}.
\]

Thus, even without knowing the transmutation kernel \( K(x, t) \) it is possible to make use of the transmutation operator \( T \) because the images of all nonnegative integer powers of \( x \) can be calculated following Definition 2.1. This result is used in the next section for obtaining an exact representation for the kernel \( K(x, t) \) in the form of a Fourier-Legendre series (Theorem 3.3).

3 The Fourier-Legendre expansion of the transmutation kernel

Let \( P_n \) denote the Legendre polynomial of order \( n \), \( l_{k,n} \) be the corresponding coefficient of \( x^k \), that is \( P_n(x) = \sum_{k=0}^{n} l_{k,n} x^k \). Denote

\[
p_{j,k} := \int_{-1}^{1} P_j(y) y^k dy, \quad j, k \in \mathbb{N} \cup \{ 0 \}.
\]

Notice that \( p_{j,k} = 0 \) when the parities of \( j \) and \( k \) do not coincide or when \( k < j \). For any \( n \geq m \) and \( \delta \in \{ 0, 1 \} \) (see, e.g., [38]),

\[
p_{2m+\delta, 2n+\delta} = \frac{\sqrt{\pi} \Gamma(2n+1+\delta) \Gamma(2m+1+\delta)}{2^{2n+\delta} \Gamma(n-m+1) \Gamma(\frac{\delta}{2}+n+m+\delta)}.
\]
Definition 3.1. Let us introduce the following infinite system of functions $\beta_k, k = 0, 1, \ldots$ defined recursively as follows

$$\beta_0(x) = \frac{f(x) - 1}{2}, \quad \beta_1(x) = \frac{3}{2} \left(\frac{\varphi_1(x)}{x} - 1\right),$$

for any even $k > 0,$

$$\beta_k(x) = \frac{1}{p_{kk}} \left(\frac{\varphi_k(x)}{x^k} - 1 - \sum_{j=0}^{k-2} p_{jk} \beta_j(x)\right),$$

and for any odd $k > 1,$

$$\beta_k(x) = \frac{1}{p_{kk}} \left(\frac{\varphi_k(x)}{x^k} - 1 - \sum_{j=1}^{k-2} p_{jk} \beta_j(x)\right).$$

Below we show that the functions $\beta_k$ admit the following direct definition as well

$$\beta_n(x) = \frac{2n + 1}{2} \left(\sum_{k=0}^{n} \frac{l_{k,n} \varphi_k(x)}{x^k} - 1\right). \quad (3.1)$$

Theorem 3.2. The transmutation kernel $K(x,t)$ from Theorem 2.3 has the form

$$K(x,t) = \sum_{j=0}^{\infty} \frac{\beta_j(x)}{x} P_j \left(\frac{t}{x}\right) \quad (3.2)$$

where for every $x \in (0,b]$ the series converges uniformly with respect to $t \in [-x,x].$

Proof. Since $K \in C^1([-b,b] \times [-b,b]),$ for any $x \in (0,b]$ it admits (see, e.g., [42]) a uniformly convergent Fourier-Legendre series of the form $\sum_{j=0}^{\infty} A_j(x) P_j \left(\frac{t}{x}\right)$ where for convenience we consider $A_j(x) = \frac{\alpha_j(x)}{x}.$ Substitution of this series into (2.6) gives us the equality

$$\varphi_k(x) = x^k + x^k \sum_{j=0}^{\infty} \frac{\alpha_j(x)}{x} \int_{-x}^{x} P_j \left(\frac{t}{x}\right) \left(\frac{t}{x}\right)^k dt$$

for any $k = 0, 1, 2, \ldots.$ The change of the variable $y := t/x$ leads to the equality

$$\varphi_k(x) = x^k \left(1 + \sum_{j=0}^{\infty} \frac{\alpha_j(x)}{x} \int_{-1}^{1} P_j(y) y^k dy\right) = x^k \left(1 + \sum_{j=0}^{k} p_{jk} \alpha_j(x)\right).$$

Solution of this system of equations leads to the conclusion $\alpha_j = \beta_j$ defined by the recursive formulas from Definition 3.1 and hence to (3.2).

Moreover, multiplying (3.2) by $P_n \left(\frac{t}{x}\right)$ and integrating we obtain

$$\int_{-x}^{x} K(x,t) P_n \left(\frac{t}{x}\right) dt = \sum_{j=0}^{\infty} \frac{\beta_j(x)}{x} \int_{-x}^{x} P_j \left(\frac{t}{x}\right) P_n \left(\frac{t}{x}\right) dt = \frac{2}{2n+1} \beta_n(x). \quad (3.3)$$

Hence

$$\beta_n(x) = \frac{2n + 1}{2} \int_{-x}^{x} K(x,t) P_n \left(\frac{t}{x}\right) dt = \frac{2n + 1}{2} \sum_{k=0}^{n} \int_{-x}^{x} K(x,t) l_{k,n} \left(\frac{t}{x}\right)^k dt$$

$$= \frac{2n + 1}{2} \sum_{k=0}^{n} l_{k,n} \int_{-x}^{x} K(x,t) t^k dt = \frac{2n + 1}{2} \sum_{k=0}^{n} l_{k,n} \frac{x^k}{x^k} (T[x^k] - x^k).$$

Using Proposition 2.4 we obtain

$$\beta_n(x) = \frac{2n + 1}{2} \sum_{k=0}^{n} l_{k,n} \frac{x^k}{x^k} (\varphi_k(x) - x^k)$$

from where (3.1) follows due to the fact that $P_n(1) = 1.$
In the next two theorems we establish a relation between the rate of convergence of partial sums of the series \((3.2)\) and the smoothness of the potential \(q\). Recall that for \(q \in C^{(p)}[0,b]\) the integral kernel \(K\) is \(p+1\) times continuously differentiable with respect to each variable \([35, \S 2]\) justifying definition \((3.4)\).

We will denote the partial sum of the series \((3.2)\) by

\[
K_N(x, t) := \sum_{j=0}^{N} \frac{\beta_j(x)}{x} P_j \left( \frac{t}{x} \right).
\]

**Theorem 3.3.** Suppose that \(q \in C^{(p)}[0,b]\) and define

\[
M := \max_{0 \leq x \leq b, \ |t| \leq x} |\partial_t^{p+1} K(x, t)|.
\]

Then for all \(N > p, 0 < x \leq b\), and \(|t| \leq x\)

\[
|K(x, t) - K_N(x, t)| \leq \frac{c_p M x^{p+1}}{N^{p+1/2}},
\]

where the constant \(c_p\) does not depend on \(q\) and \(N\).

**Proof.** The following estimate for the remainder of the Fourier-Legendre series for a function \(g \in C^{(p+1)}[-1,1]\) is known (see the proof of Theorem 4.10 from \([42]\) together with \([33, \S 5.2.1]\)): for all \(N > p+1\)

\[
\max \{ |g(x) - g_N(x)| \leq \frac{c_{p+1} M_g}{N^{p+1/2}},
\]

where \(g_N(x) = \sum_{k=0}^{N} a_k P_k(x)\) is a partial sum of the Fourier-Legendre series of the function \(g\), \(M_g := \max_{[-1,1]} |g^{(p+1)}(x)|\) and the constant \(c_{p+1}\) does not depend on \(g\) and \(N\).

For each \(x \in (0,b]\) let us consider a function \(g(y) := K(x,xy), y \in [-1,1]\). Since the integral kernel \(K\) is \(p+1\) times continuously differentiable with respect to the second variable, \(g \in C^{(p+1)}[-1,1]\), and \(g^{(p+1)}(y) = x^{p+1} \partial_t^{p+1} K(x, t)\big|_{t=xy}\). Hence

\[
\max_{[-1,1]} |g^{(p+1)}(y)| \leq x^{p+1} \max_{y \in [-1,1]} \left| \partial_t^{p+1} K(x, t)\big|_{t=xy} \right| \leq x^{p+1} M.
\]

Now \((3.5)\) follows directly from \((3.6)\) and \((3.7)\) noting that \(\sum_{j=0}^{N} \frac{\beta_j(x)}{x} P_j(y)\) is a partial sum of the Fourier-Legendre series for the function \(g(y)\).

**Remark 3.4.** Actually, the value of the integral kernel \(K\) at some point \((x,t), x > 0\), depends only on values of the potential \(q\) on the segment \([0,x]\) and does not depend on values of \(q\) on \([x,b]\), which can be deduced, e.g., from \((3.5)\). Therefore the estimate \((3.5)\) remains valid if we change all entries of \(b\) in Theorem \(3.3\) by some \(b'\) such that \(x \leq b' \leq b\).

The next theorem partially inverts the result of Theorem \(3.3\). We need the following auxiliary result on the connection between the smoothness of the function \(K(x, \cdot)\) (for a fixed \(x\)) and the smoothness of the potential \(q\). Even though similar results are well known, we are not aware of a precise reference. In any case, the statement of the lemma can be easily verified using the integral equation satisfied by \(K\) (see, e.g., \([33, \Sect. 1.2] and [35, \S 2]\))

\[
K(x, t) = \frac{h}{2} + \frac{1}{2} \int_0^\infty q(s) \, ds + \int_0^\infty \int_0^\infty q(\alpha + \beta) K(\alpha + \beta, \alpha - \beta) \, d\beta \, d\alpha.
\]

**Lemma 3.5.** Let \(x > 0\) be fixed. Suppose that there exists an integer \(p \geq 1\) such that \(K(x, \cdot) \in C^{(p)}[-x,x]\). Then \(q \in C^{(p-1)}[0,x]\). If additionally \(K(x, \cdot) \in C^{(r)}(-x,x)\) for some \(p < r \leq 2p + 1\), then \(q \in C^{(r-1)}(0,x)\).
Theorem 3.6. Let \( x > 0 \) be fixed. Suppose that there exist an integer \( p \geq 2 \) and the constants \( c \) and \( \varepsilon > 0 \) such that for all \( N > p + 1 \) and all \( t, |t| \leq x \),

\[
|K(x, t) - K_N(x, t)| \leq \frac{c}{N^{p+\varepsilon}}. \tag{3.9}
\]

Then \( q \in C^{([p/2]-1)[0, x]} \cap C^{(p-1)}(0, x) \), where \([a]\) denotes the largest integer less or equal to \( a \).

**Proof.** The sum \( \sum_{j=0}^{\infty} \frac{\sin (\omega x)}{\sqrt{x}} \) is a polynomial of degree at most \( N \) approximating the function \( K(x, \cdot) \). That is, the inequality (3.9) provides an upper bound for the best uniform approximation of the function \( K(x, \cdot) \) by degree \( N \) polynomials. The application of the inverse approximation theorem (see, e.g., [22, Theorem 31]) leads to the conclusion that \( K(x, \cdot) \in C^{(p)}(-x, x) \cap C^{[p/2]}[-x, x] \). Now the proof follows directly from Lemma 3.5. \( \square \)

4 Representation for solutions of the Schrödinger equation

**Theorem 4.1.** The solutions \( c(\omega, x) \) and \( s(\omega, x) \) of equation (1.1) admit the following representations

\[
c(\omega, x) = \cos \omega x + \sqrt{\frac{2\pi}{\omega x}} \sum_{n=0}^{\infty} (-1)^n \beta_{2n}(x) J_{2n+1/2}(\omega x)
\]

\[
= \cos \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n}(x) j_{2n}(\omega x) \tag{4.1}
\]

and

\[
s(\omega, x) = \sin \omega x + \sqrt{\frac{2\pi}{\omega x}} \sum_{n=0}^{\infty} (-1)^n \beta_{2n+1}(x) J_{2n+3/2}(\omega x)
\]

\[
= \sin \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n+1}(x) j_{2n+1}(\omega x) \tag{4.2}
\]

where \( j_k \) stands for the spherical Bessel function of order \( k \), the series converge uniformly with respect to \( x \) on \([0, b]\) and converge uniformly with respect to \( \omega \) on any compact subset of the complex plane of the variable \( \omega \). Moreover, for the functions

\[
c_N(\omega, x) = \cos \omega x + 2 \sum_{n=0}^{[N/2]} (-1)^n \beta_{2n}(x) j_{2n}(\omega x) \tag{4.3}
\]

and

\[
s_N(\omega, x) = \sin \omega x + 2 \sum_{n=0}^{[(N-1)/2]} (-1)^n \beta_{2n+1}(x) j_{2n+1}(\omega x) \tag{4.4}
\]

the following estimates hold

\[
|c(\omega, x) - c_N(\omega, x)| \leq 2|x| \varepsilon_N(x) \quad \text{and} \quad |s(\omega, x) - s_N(\omega, x)| \leq 2|x| \varepsilon_N(x) \tag{4.5}
\]

for any \( \omega \in \mathbb{R}, \omega \neq 0 \), and

\[
|c(\omega, x) - c_N(\omega, x)| \leq 2\varepsilon_N(x) \frac{\sinh(Cx)}{C} \quad \text{and} \quad |s(\omega, x) - s_N(\omega, x)| \leq 2\varepsilon_N(x) \frac{\sinh(Cx)}{C} \tag{4.6}
\]

for any \( \omega \in \mathbb{C}, \omega \neq 0 \) belonging to the strip \( |\text{Im} \omega| \leq C, C \geq 0 \), where \( \varepsilon_N \) is a sufficiently small nonnegative function such that \( |K(x, t) - K_N(x, t)| \leq \varepsilon_N(x) \) which exists due to Theorem 5.2 (an estimate for \( \varepsilon_N(x) \) is presented in (3.3)).
Proof. Substitution of $K(x,t)$ in the form of the series (3.2) into (2.5) leads to the equalities
\[ c(\omega, x) = \cos \omega x + \sum_{j=0}^{\infty} \frac{\beta_j(x)}{x} \int_{-\infty}^{\infty} P_j \left( \frac{t}{x} \right) \cos \omega t \, dt = \cos \omega x + \sum_{j=0}^{\infty} \beta_j(x) \int_{-1}^{1} P_j(y) \cos (\omega xy) \, dy \]
and
\[ s(\omega, x) = \sin \omega x + \sum_{j=0}^{\infty} \beta_j(x) \int_{-1}^{1} P_j(y) \sin (\omega xy) \, dy. \]
Using formula 2.17.7 from [38, p. 433],
\[ \int_0^a \left\{ \frac{P_{2n+1}(\xi)}{P_{2n}(\xi)} \cdot \sin \gamma y \right\} dy = (-1)^n \sqrt{\frac{\pi \alpha}{2b}} J_{2n+\delta}(ab), \delta = \left\{ \begin{array}{ll} 1 & , a > 0, \end{array} \right. \]
we obtain the representations (4.1) and (4.2).

The convergence of the series with respect to $\omega$ can be established using the fact that for each $x$ the series represent the Neumann series (see, e.g., [47] and [48]). Indeed, the function $\omega (c(\omega, x) - \cos \omega x)$ regarded as a function of a complex variable $\omega$ is entire and as the radius of convergence of the Neumann series coincides with the radius of convergence of its associated power series (obtained from the SPPS representation) we obtain that the series (4.1) and (4.2) converge uniformly on any compact subset of the complex plane of the variable $\omega$.

Consider a complex $\omega \neq 0$ belonging to the strip $|\text{Im}\omega| \leq C$. We obtain
\[ |c(\omega, x) - c_N(\omega, x)| \leq \int_0^x |K(x,t) - K_N(x,t)| |\cos \omega t| \, dt \leq 2\varepsilon_N(x) \int_0^x |\cos \omega t| \, dt \]
\[ \leq \varepsilon_N(x) \int_0^x \left( e^{\text{Im}\omega t} + e^{-\text{Im}\omega t} \right) \, dt = 2\varepsilon_N(x) \int_0^x \cosh (|\text{Im}\omega| \, t) \, dt = \frac{2\varepsilon_N(x) \sinh (|\text{Im}\omega| \, x)}{|\text{Im}\omega|}. \]
Since the function $\sinh(\xi x)/\xi$ is monotonically increasing with respect to both variables when $\xi, x \geq 0$, we obtain the required inequality (4.6). The second inequality in (4.6) and the inequalities (4.5) are proved similarly.

The uniform convergence of the series (4.1) and (4.2) with respect to the variable $x$ follows directly from the inequalities (4.5) and (4.6) and estimate (3.5) valid at least for $p = 0$.

**Remark 4.2.** The inequalities (4.5) and (4.6) are of particular importance when using representations (4.1) and (4.2) for solving spectral problems for (1.1) because they guarantee a uniform ($\omega$-independent) approximation of eigendata (see [50, Proposition 7.1]) which is illustrated by numerical experiments in Section 7.

**Remark 4.3.** In [27] another representation for solutions of (1.1) was obtained in the form of Neumann series of Bessel functions. It was based on the representation of the functions $\sin \omega x$ and $\cos \omega x$ as series in terms of Chebyshev polynomials. To the difference of the result of Theorem 4.1 that idea did not lead to an approximation of the solutions uniform with respect to $\omega$.

Note that the numbers $j_k(z)$ for fixed $z$ rapidly decrease as $k \to \infty$, see, e.g., [1] (9.1.62)]. Hence, the convergence rate of the series (4.1) and (4.2) for any fixed $\omega$ (and for bounded subsets $\Omega \subset \mathbb{C}$) is, in fact, exponential.

**Proposition 4.4.** Let $x > 0$ be fixed and $\omega \in \mathbb{C}$ satisfy $|\omega| \leq \omega_0$. Suppose that $q \in C^p(0, b]$ for some $p \in \mathbb{N}_0$. Then for all $N > \max\{\omega_0 x, p\}/2$ the remainders of the series (4.1) and (4.2) satisfy
\[ |c(\omega, x) - c_{2N}(\omega, x)| = |c(\omega, x) - c_{2N+1}(\omega, x)| \leq \frac{c x^{p+2} e^{\text{Im}\omega x}}{(2N + 2)^{p+1/2}} \cdot \frac{1}{(2N + 2)!} \cdot \left| \frac{\omega_0 x}{2} \right|^{2N + 2}, \]
and
\[ |s(\omega, x) - s_{2N-1}(\omega, x)| = |s(\omega, x) - s_{2N}(\omega, x)| \leq \frac{c x^{p+2} e^{\text{Im}\omega x}}{(2N + 1)^{p+1/2}} \cdot \frac{1}{(2N + 1)!} \cdot \left| \frac{\omega_0 x}{2} \right|^{2N + 1}, \]
where $c$ is a constant depending on $q$ and $p$ only.
Proof. It follows from (3.3) that
\[ \beta_n(x) = \frac{2n + 1}{2} \int_{-x}^{x} K(x,t)P_n\left(\frac{t}{x}\right) \, dt = \frac{2n + 1}{2} \int_{-1}^{1} xK(x,xz)P_n(z) \, dz, \]
(4.8)
i.e., for every \( x > 0 \) the numbers \( \beta_n(x) \) are the Fourier-Legendre coefficients of the function \( g(z) := xK(x,xz) \). Since \( q \in C^p[0,b] \), the function \( g \in C^{p+1}[-1,1] \) and hence (see [20], Corollary I to Theorem XIV) and [10]
\[ |\beta_n(x)| \leq c_p V x^{p+2} n^{p+1} / 2, \quad n > p, \]
(4.9)
where \( c_p > 0 \) is a universal constant and \( V = \max_{x \leq b, |t| \leq x} |\partial_t^{p+1} K(x,t)| \). Combining the inequality (4.9) with the inequality [1, (9.1.62)]
\[ |j_n(z)| \leq \sqrt{\pi} |z|^{n} e^{1mz} \]
one easily obtains the announced estimates. \qed

5 Representation for derivatives of solutions

Differentiation of the equalities (2.5) with respect to \( x \) and the Goursat conditions
\[ K(x,x) = \frac{h}{2} + \frac{1}{2} \int_{0}^{x} q(s) \, ds, \quad K(x,-x) = \frac{h}{2}, \quad 0 \leq x \leq b \]
(5.1)
give us the relations
\[ c'(\omega, x) = -\omega \sin \omega x + \int_{-x}^{x} K_1(x,t) \cos \omega t \, dt + \left( h + \frac{1}{2} \int_{0}^{x} q(s) \, ds \right) \cos \omega x \]
(5.2)
and
\[ s'(\omega, x) = \omega \cos \omega x + \int_{-x}^{x} K_1(x,t) \sin \omega t \, dt + \frac{1}{2} \left( \int_{0}^{x} q(s) \, ds \right) \sin \omega x. \]
(5.3)
Here \( K_1(x,t) \) is the derivative of \( K(x,t) \) with respect to the first variable. To obtain a convenient representation for the kernel \( K_1(x,t) \) we can apply a procedure similar to that from Section 3. Let us seek \( K_1(x,t) \) in the form
\[ K_1(x,t) = \sum_{j=0}^{\infty} \gamma_j(x) P_j\left(\frac{t}{x}\right). \]
(5.4)
Then analogously to (3.3) we have
\[ \gamma_n(x) = \frac{2n + 1}{2} \int_{-x}^{x} K_1(x,t)P_n\left(\frac{t}{x}\right) \, dt. \]
(5.5)

Differentiation of (2.6) (and the use of (5.1)) gives us the relations
\[ \int_{-x}^{x} K_1(x,t) t^k \, dt = \varphi_k(x) - kx^{k-1} - \frac{1}{2} \left( 1 + (-1)^k \right) h + \int_{0}^{x} q(s) \, ds \] \( x^k. \)
Using (5.5) we obtain then
\[ \gamma_n(x) = \frac{2n + 1}{2} \sum_{k=0}^{n} \frac{l_{k,n}}{x^k} \int_{-x}^{x} K_1(x,t) t^k \, dt \]
\[ = \frac{2n + 1}{2} \left( \sum_{k=0}^{n} \frac{l_{k,n}\varphi_k'(x)}{x^k} - \frac{n(n+1)}{2x} - \frac{1}{2} \int_{0}^{x} q(s) \, ds - \frac{h}{2} (1 + (-1)^n) \right) \]
(5.6)
where several elementary properties of Legendre polynomials (such as $\sum_{k=0}^n l_{k,n} = P_n(1) = 1$ and $\sum_{k=1}^n kl_{k,n} = P_n'(1) = n(n+1)$) were employed.

Finally, if $f$ does not have zeros on $[0,b]$ (such $f$ always exists \[20\] Remark 5) and \[17\], the derivatives $\varphi'_{k}$ can be calculated by the formula

$$\varphi'_{k} = k\psi_{k-1} + \frac{f'}{f}\varphi_{k}$$

which follows directly from Definition \[21\]. Otherwise it is convenient to use the formulas from \[28\].

In general, $K_1$ is a continuous function with respect to both variables however we cannot guarantee additional smoothness of $K_1$ as function of $t$ (moreover, similarly to Lemma \[35\] it is possible to show that belonging of $K_1(x,\cdot)$ to some class Lip $\alpha$ implies $q \in$ Lip $\alpha$). And it is known that the Fourier-Legendre series of a continuous function may not converge to the function even pointwise. Nevertheless, the series always converges to the function in the $L_2$ norm.

Denote by $K_{1,N}$ the partial sum of the series \[54\],

$$K_{1,N}(x,t) = \sum_{j=0}^{N} \frac{\gamma_j(x)}{x} P_j \left( \frac{t}{x} \right).$$

Below we prove some estimates for the remainder $K_1 - K_{1,N}$ with explicit dependence on $x$.

Let $q \in C^{(p)}[0,b]$. Then $K_1$ is $p$ times continuously differentiable with respect to $t$ which justifies the existence of the following constants. Define

$$M_p := \max_{0 \leq x \leq b, |t| \leq x} |\partial^K K_1(x,t)|.$$

and

$$k_0(\delta) := \sup_{0 \leq t \leq \delta} \sup_{0 \leq x \leq b} \sup_{t_1,t_2 \in [0,\delta]:|t_1-t_2| \leq \tau}|K_1(x,t_1) - K_1(x,t_2)|.$$

Since the kernel $K_1$ is a continuous function in the domain $0 \leq x \leq b, |t| \leq x$, we have $k_0(\delta) = 0$, $\delta \to 0$.

**Proposition 5.1.** Suppose that $q \in C^{(p)}[0,b]$. Then for $p = 0$, $N \in \mathbb{N}$ and each $x \in (0,b]$

$$\|K_1(x,\cdot) - K_{1,N}(x,\cdot)\|_{L_2[-x,x]} \leq c_0 \sqrt{x} \cdot k_0 \left( \frac{x}{n} \right) \leq c_0 \sqrt{x} \cdot k_0 \left( \frac{b}{n} \right) = o(1), \quad N \to \infty, \quad (5.7)$$

and for $p \geq 1$, $0 \leq x \leq b, |t| \leq x$

$$|K_1(x,t) - K_{1,N}(x,t)| \leq \frac{c_p M_x x^p}{N^{p-1/2}}, \quad N > p, \quad (5.8)$$

where the constants $c_0$ and $c_p$ do not depend on $q$ and $N$.

**Proof.** Theorem 6.2 from \[14\] states that for a function $f \in W^r L_2([-1,1],r \in \mathbb{N}_0)$, the error $E_n(f)_2$ of the best approximation of $f$ by polynomials of degree not exceeding $n$ (which in the case of $L_2$ norm coincides with the partial sum of the Fourier-Legendre series of $f$) satisfies

$$E_n(f)_2 \leq c_r n^{-r} \omega(f^{(r)},1/n)_2, \quad (5.9)$$

where the constant $c_r$ does not depend on $f$ and $\omega$ is the modulus of continuity defined for a function $g \in L_2[a,b]$ as

$$\omega(g,t)_2 := \sup_{0 \leq \tau \leq t} \|g(x + \tau) - g(x)\|_{L_2[a,b-\tau]}.$$  

For a fixed $x > 0$ consider a function $g(y) := K_1(x,xy)$, $-1 \leq y \leq 1$. Then

$$\omega \left( g, \frac{1}{n} \right)_2 = \sup_{0 \leq \tau \leq 1/n} \left( \int_{-1}^{-1} |g(y + \tau) - g(y)|^2 dy \right)^{1/2} \leq \sup_{0 \leq \tau \leq 1/n} \sqrt{2} k_0(x\tau) \leq \sqrt{2} k_0 \left( \frac{x}{n} \right). \quad (5.10)$$
Note that
\[ \|K_1(x, \cdot) - K_{1,N}(x, \cdot)\|_{L_2[-x,x]} = \sqrt{x}\|g - g_N\|_{L_2[-1,1]} = \sqrt{x}E_0(g)_2, \]
where \( g_N \) is the partial sum of the Fourier-Legendre series for the function \( g \). Combining the last equality with (5.9) for \( r = 0 \) and with (5.10) we obtain (5.7).

The second inequality (5.8) can be obtained similarly to the proof of Theorem 3.3.

**Proposition 5.2.** The derivatives of the solutions \( c(\omega, x) \) and \( s(\omega, x) \) of equation (1.1) admit the following representations

\[
c'(\omega, x) = -\omega \sin \omega x + \left( h + \frac{1}{2} \int_0^x q(s) \, ds \right) \cos \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \gamma_{2n}(x) j_{2n}(\omega x) \tag{5.11}
\]

and

\[
s'(\omega, x) = \omega \cos \omega x + \frac{1}{2} \left( \int_0^x q(s) \, ds \right) \sin \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \gamma_{2n+1}(x) j_{2n+1}(\omega x) \tag{5.12}
\]

where \( \gamma_k \) are defined by (5.6). The series converge uniformly for any \( x \) from \([0, b]\) and converge uniformly with respect to \( \omega \) on any compact subset of the complex plane of the variable \( \omega \).

**Proof.** The proof of these representations follows from (5.2) and (5.3) by substitution of (5.4) and similar procedure as that from the proof of Theorem 4.1. The uniform convergence of the series with respect to \( x \) follows from Proposition 5.1 and Cauchy-Schwarz inequality. The uniform convergence with respect to \( \omega \) is proved analogously to Theorem 4.1.

**Remark 5.3.** Consider the approximations of the derivatives of the solutions

\[
c_N(\omega, x) = -\omega \sin \omega x + \left( h + \frac{1}{2} \int_0^x q(s) \, ds \right) \cos \omega x + 2 \sum_{n=0}^{[N/2]} (-1)^n \gamma_{2n}(x) j_{2n}(\omega x) \tag{5.13}
\]

and

\[
s_N(\omega, x) = \omega \cos \omega x + \frac{1}{2} \left( \int_0^x q(s) \, ds \right) \sin \omega x + 2 \sum_{n=0}^{[N-1]/2} (-1)^n \gamma_{2n+1}(x) j_{2n+1}(\omega x). \tag{5.14}
\]

Let \( \varepsilon_N \) be a sufficiently small nonnegative function such that \( |K_1(x, t) - K_{1,N}(x, t)| \leq \varepsilon_N(x) \). Then for the differences between \( c'(\omega, x) \) and \( c_N(\omega, x) \), as well as between \( s'(\omega, x) \) and \( s_N(\omega, x) \), we obtain exactly the same estimates as (4.15) and (4.16). Their proof is analogous.

**Remark 5.4.** The representations proposed for solutions and their derivatives are not limited to continuous potentials \( q \). Consideration of the convergence of the series (4.2) and (5.1) in the \( L_2 \) norm is possible for wider classes of potentials, up to \( q \in W_2^{-1}(0, b) \), see [18, 19] for the definitions and construction of transmutation operators in that case.

### 6 A sequence of equations for \( \beta_k \) and \( \gamma_k \)

In this section we develop another recursive procedure for calculating the functions \( \beta_k \) and \( \gamma_k \). It is based on the substitution of the solutions \( c(\omega, x) \) and \( s(\omega, x) \) in the form (4.1) and (4.2) into equation (1.1).

One of the advantages of this procedure is the improved stability for numerical calculations. For example, the first formula from Definition 3.1 includes the term

\[
\frac{p_{0k}}{p_{kk}} = \frac{(2k + 1)!}{k!(k + 1)!2^k} \beta_0 \sim \frac{2^{k+1}}{\sqrt{\pi k}} \beta_0,
\]

where we applied formulas from [12, Chap. 4] and Stirling’s formula. Hence even the smallest error in the computation of \( \beta_0 \) leads to exponentially growing errors in subsequent \( \beta_k \)'s. Errors in other previous \( \beta_m \)'s are get multiplied as well. On the other hand, for any \( x \) the functions \( \beta_k(x)/x \) are the Fourier-Legendre coefficients of a smooth function \( K(x, xt) \) and hence tend to zero as \( k \to \infty \) (see also Remark 7.1). This
explains why using Definition 3.1 only a limited number of the functions \( \beta_k \) can be evaluated numerically. The procedure developed in this section presents different recurrent formulas which allowed more functions \( \beta_k \) to be evaluated numerically in all experiments performed, see Example 7.2 for details.

Let us start with the solution \( c(\omega, x) \) (see Theorem 1.1). Analogous formulas for \( s(\omega, x) \) are given below. We proceed formally and at the end of this section justify for the case \( q \in C^\infty[0, b] \) the possibility to differentiate termwise all the series and explain why the final formulas remain valid for the general case. Differentiating the solution \( c(\omega, x) \) twice, using the formulas \( j_k'(z) = -j_{k+1}(z) + \frac{k}{2} j_k(z) \), \( k = 0, 1, \ldots \) (for the first derivative) and \( j_k''(z) = j_{k-1}(z) - \frac{k+1}{2} j_k(z) \), \( k = 1, 2, \ldots \) (for the second derivative) and substituting into (1.1) leads us to the equality

\[
2 \sum_{n=0}^{\infty} (-1)^n \left[ j_{2n}(\omega x) \left( \frac{\beta''_{2n}(x)}{4n} + \frac{2n(2n-1)}{x^2} \beta_{2n}(x) \right) + j_{2n+1}(\omega x) \left( -2\omega \beta''_{2n}(x) + \frac{2\omega}{x} \beta_{2n}(x) \right) \right] = q(x) \left( \cos \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n}(x) j_{2n}(\omega x) \right).
\]

Combining the terms containing \( j_0(\omega x) \) and using \( q(x) = 2(\beta''_0(x) - q(x)\beta_0(x)) \) we obtain

\[
(\cos \omega x - j_0(\omega x)) (\beta''_0(x) - q(x)\beta_0(x)) = -2\omega \sum_{n=0}^{\infty} (-1)^n j_{2n+1}(\omega x) \left( \beta''_{2n}(x) - \frac{1}{x} \beta_{2n}(x) \right) + \sum_{n=1}^{\infty} (-1)^n j_{2n}(\omega x) \left( \beta''_{2n}(x) + \frac{4n}{x} \beta'_{2n}(x) + \frac{2n(2n-1)}{x^2} \beta_{2n}(x) - q(x)\beta_{2n}(x) \right).
\]

The second series can be expressed in the terms of odd index spherical Bessel functions using the equality

\[
j_{2n}(\omega x) = \frac{\omega x}{4n+1} \left( j_{2n-1}(\omega x) + j_{2n+1}(\omega x) \right).
\]

Note additionally that

\[
\cos \omega x - j_0(\omega x) = \omega x \cdot j_1(\omega x).
\]

Applying (6.3) and (6.2) to (6.1) and dividing by \( \omega x \) one can see that (6.1) can be written as

\[
\sum_{n=1}^{\infty} \alpha_n(x) j_{2n-1}(\omega x) = 0,
\]

where

\[
\alpha_n(x) = (-1)^n \left[ \frac{1}{4n+1} \left( \beta''_{2n}(x) + \frac{4n}{x} \beta'_{2n}(x) + \left( \frac{2n(2n-1)}{x^2} - q(x) \right) \beta_{2n}(x) \right) - \frac{1}{4n-3} \left( \beta''_{2(n-1)}(x) + \frac{4(n-1)}{x} \beta'_{2(n-1)}(x) + \left( \frac{2(n-1)(2(n-1)-1)}{x^2} - q(x) \right) \beta_{2(n-1)}(x) \right) + 2 \left( \frac{1}{x} \beta'_{2(n-1)}(x) \right) \right].
\]

Multiplying the equality (6.1) by \( j_{2m-1}(\omega x) \), \( m = 1, 2, \ldots \), integrating with respect to \( \omega \) from 0 to \( \infty \) and using the integral

\[
\int_0^{\infty} j_{\nu+2m}(y) j_{\nu+2m}(y) dy = 0
\]

for \( n, m \in \mathbb{Z} \) with \( n \neq m \) and \( m + n + \nu > -1/2 \) (c.f., [1, Formula 11.4.6]) we obtain that all coefficients \( \alpha_n \) are identically equal to zero.

In order to simplify the equations \( \alpha_n(x) = 0 \), \( n = 1, 2, \ldots \), consider the functions

\[
\sigma_{2n}(x) := x^{2n} \beta_{2n}(x), \quad n = 0, 1, \ldots .
\]
Then equations $\alpha_n(x) = 0$ take the form

$$
\sigma''_{2n}(x) - q(x)\sigma_{2n}(x) = \frac{4n + 1}{4n - 3} \frac{x^2}{4} \left( \sigma''_{2(n-1)}(x) - q(x)\sigma_{2(n-1)}(x) \right) - 2 (4n + 1) x \left( \sigma'_{2(n-1)}(x) - \frac{2n - 1}{x} \sigma_{2(n-1)}(x) \right). \tag{6.6}
$$

Equations similar to (6.6) can be derived also for the odd coefficients. Calculation similar to that for $c(\omega, x)$ leads to the equality

$$
\frac{q(x) \omega x}{2} = \sum_{n=0}^{\infty} (-1)^n \left[ \frac{j_{2n}^{(2)}(\omega x)}{4n + 3} \left( \beta''_{2n+1}(x) + \frac{2(2n + 1)}{x} \beta'_{2n+1}(x) + \left( \frac{2n(2n + 1)}{x^2} - q(x) \right) \beta_{2n+1}(x) \right) \\
+ \frac{j_{2n+2}^{(2)}(\omega x)}{4n + 3} \left( \beta''_{2n+1}(x) + \frac{2(2n + 1)}{x} \beta'_{2n+1}(x) + \left( \frac{2n(2n + 1)}{x^2} - q(x) \right) \beta_{2n+1}(x) \right) \\
- 2 j_{2n+2}^{(2)}(\omega x) \left( \frac{1}{x} \beta'_{2n+1}(x) - \frac{1}{x^2} \beta_{2n+1}(x) \right) \right].
$$

Noting that $\sin(\omega x)/\omega x = j_0(\omega x)$ one can see that the last equality is of the form

$$
\sum_{n=0}^{\infty} \alpha_n(x) j_{2n}(\omega x) = 0,
$$

where

$$
\alpha_n(x) = (-1)^n \left[ \frac{1}{4n + 3} \left( \beta''_{2n+1}(x) + \frac{2(2n + 1)}{x} \beta'_{2n+1}(x) + \left( \frac{2n(2n + 1)}{x^2} - q(x) \right) \beta_{2n+1}(x) \right) \\
- \frac{1}{4n - 1} \left( \beta''_{2n-1}(x) + \frac{2(2n - 1)}{x} \beta'_{2n-1}(x) + \left( \frac{(2n - 2)(2n - 1)}{x^2} - q(x) \right) \beta_{2n-1}(x) \right) \\
+ 2 \left( \frac{1}{x} \beta'_{2n-1}(x) - \frac{1}{x^2} \beta_{2n-1}(x) \right) \right]
$$

and we have taken $\beta_{-1} := 1/2$ to simplify notations for $n = 0$. Applying the integral [6.5] one obtains the relations $\alpha_n \equiv 0$ for $n = 0, 1, 2, \ldots$. Introducing $\sigma_{2n+1} = x^{2n+1} \beta_{2n+1}(x)$ we rewrite them in the form

$$
\frac{1}{4n + 3} \left( \sigma''_{2n+1}(x) - q(x)\sigma_{2n+1}(x) \right) = \frac{x^2}{4n - 1} \left( \sigma''_{2n-1}(x) - q(x)\sigma_{2n-1}(x) \right) - 2x \left( \sigma'_{2n-1}(x) - \frac{2n}{x} \sigma_{2n-1}(x) \right).
$$

Combining the even with the odd cases we obtain the following sequence of equations to find coefficients $\beta_n(x) = x^{-n}\sigma_n(x)$ for the representations of solutions

$$
\frac{1}{2n + 1} \left( \sigma''_n(x) - q(x)\sigma_n(x) \right) = \frac{x^2}{2n - 3} \left( \sigma''_{n-2}(x) - q(x)\sigma_{n-2}(x) \right) - 2x \left( \sigma'_{n-2}(x) - \frac{n-1}{x} \sigma_{n-2}(x) \right). \tag{6.7}
$$

To obtain the equations for the coefficients $\gamma_k$ one has to compare (5.11) and (5.12) with the derivatives of (4.1) and (4.2) and proceed similarly to the previous cases. As a result, the following relations can be obtained

$$
\begin{align*}
\gamma_0(x) &= \beta'_0(x) - \frac{h}{2} - \frac{1}{4} \int_0^x q(s) \, ds, \\
\gamma_1(x) &= \frac{1}{x} \beta_1(x) + \beta'_1(x) - \frac{3}{4} \int_0^x q(s) \, ds, \\
\gamma_n(x) &= \frac{n}{x} \beta_n(x) + \beta'_n(x) + \frac{2n + 1}{2n - 3} \left( \gamma_{n-2}(x) - \beta'_{n-2}(x) + \frac{n-1}{x} \beta_{n-2}(x) \right), \quad n = 2, 3, \ldots \tag{6.8}
\end{align*}
$$
Note that the last formula holds for \( n = 1 \) as well if we define \( \gamma_{-1} := \frac{1}{2} \int_0^x q(s) \, ds \). Introducing notations \( \tau_n(x) := x^n \gamma_n(x) \) we can rewrite equation (6.8) in terms of the functions \( \sigma_n \).

\[
\tau_n(x) = \sigma_n'(x) + \frac{2n+1}{2n-3} x^2 (\tau_{n-2}(x) - \sigma_n'(x)) + (2n+1)x \sigma_{n-2}(x).
\]  

(6.9)

Hence the construction of the functions \( \beta_n \) and \( \gamma_n \) for \( n = 1, 2, \ldots \) reduces to solving of a recurrent sequence of inhomogeneous Schrödinger equations (6.7) having the form

\[
\sigma_n''(x) - q(x) \sigma_n(x) = h_n(x)
\]

(6.10)

with the initial conditions \( \sigma_n(0) = \sigma_n'(0) = 0 \).

Thus, the following statement is proved.

**Proposition 6.1.** The functions \( \sigma_n(x) := x^n \beta_n(x) \) where \( \beta_n \) are the coefficients from (4.11) and (4.2) satisfy the sequence of recurrent differential equations (6.7) for \( n = 1, 2, \ldots \) with the initial conditions \( \sigma_n(0) = \sigma_n'(0) = 0 \) and with the first functions given by \( \beta_{-1} := 1/2 \) and \( \beta_0 = (f-1)/2 \). The functions \( \tau_n(x) := x^n \gamma_n(x) \) where \( \gamma_n \) are the coefficients from (5.11) and (5.12) are given by the sequence of recurrent relations (6.9) with the first functions given by \( \gamma_{-1} := \frac{1}{2} \int_0^x q(s) \, ds \) and \( \gamma_0 = \frac{f-1}{2} - \frac{1}{4} \int_0^x q(s) \, ds \).

**Remark 6.2.** The values \( \sigma_1(x) = \frac{1}{2} (\varphi_1(x) - x) \) and \( \tau_1(x) = \frac{3}{2} \left( \frac{\varphi_1(x)}{f} + 1 - \frac{1}{2} \int_0^x q(s) \, ds \right) \) can also be used as the initial values for Proposition 6.1.

**Remark 6.3.** Let \( L := \partial^2 - q(x) \). Equations (6.7) and (6.8) can be written in the following somewhat more symmetric form

\[
\frac{1}{x^n} L [x^n \beta_n(x)] = \frac{2n+1}{2n-3} x^{n-1} \left[ \beta_{n-2}(x) \right],
\]

\[
\gamma_n(x) - \frac{1}{x^n} (x^n \beta_n(x))' = \frac{2n+1}{2n-3} \left[ \gamma_{n-2}(x) - x^{n-1} \left( \frac{\beta_{n-2}(x)}{x^n} \right)' \right] .
\]

The solution of the inhomogeneous Schrödinger equations (6.10) with the initial conditions \( \sigma_n(0) = \sigma_n'(0) = 0 \) can be taken in the form (c.f., [26])

\[
\sigma_n(x) = f(x) \int_0^x \left( \int_0^{f(t)} \int_0^{f(t) h_n(t)} dt \right) ds .
\]

Substituting the right-hand side from equation (6.7) and performing several integrations by parts to get rid of the derivatives of the function \( \sigma_{n-2} \) under the integral signs we obtain the following recurrent formulas for the functions \( \sigma_n \) and \( \tau_n \).

\[
\eta_n(x) = \int_0^x (t f'(t) + (n-1)f(t)) \sigma_{n-2}(t) \, dt , \quad \theta_n(x) = \int_0^x \frac{1}{f^2(t)} (\eta_n(t) - t f(t) \sigma_{n-2}(t)) \, dt ,
\]

\[
\tau_n(x) = \frac{2n+1}{2n-3} \left[ x^2 \tau_{n-2}(x) + c_n f(x) \theta_n(x) \right],
\]

\[
\sigma_n(x) = 2n+1 \left[ x^2 \sigma_{n-2}(x) + c_n f(x) \eta_n(x) \right],
\]

(6.11)

(6.12)

where \( c_n = 1 \) if \( n = 1 \) and \( c_n = 2(2n-1) \) otherwise.

Now we explain why the series (4.11) and (4.12) can be differentiated termwise. Suppose that \( g \in C^2[0, b] \). First, it follows from the equality \( \sum_{n=0}^{\infty} (2n+1) j_n^2(z) = 1 \) (11.1.50) and Cauchy-Schwarz inequality that a series \( \sum_{n=0}^{\infty} a_n(x) j_{2n+\delta}(\psi x) \) (where \( \delta \) is zero or one) is uniformly convergent provided that the series \( \sum_{n=0}^{\infty} a_n^2(x) / n \) is uniformly convergent. Second, it follows from [20] Corollary I to Theorem XIV and [40] that for a function \( g \in C^{(a+1)}[-1, 1] \) its Fourier-Legendre coefficients \( a_n(g) \) satisfy

\[
|a_n(g)| \leq \frac{c_p V}{n^{a+1/2}} ,
\]

(6.13)
where \( c_0 \) is a universal constant and \( V = \max_{[-1,1]} |q^{(p+1)}(x)| \).

Consider coefficients \( \beta_n \). As can be seen from (4.11), \( \beta_n \in C^2[0,b] \) (at \( x = 0 \) we define \( \beta_n \) by continuity). Moreover, \( \beta_n(x) \) are the Fourier-Legendre coefficients of the function \( xK(x,xz) \in C^{(3)}[-1,1] \) (with respect to \( z \), see (4.3)). Hence \( |\beta_n(x)| \leq c_3 n^{-5/2} \). For the derivatives we have

\[
\beta'_n(x) = \frac{2n+1}{2} \int_{-1}^{1} (K(x,xz) + xK_1(x,xz) + xzK_2(x,xz)) P_n(z) \, dz,
\]

i.e., \( \beta'_n(x) \) are the Fourier-Legendre coefficients of the function \( K(x,xz) + xK_1(x,xz) + xzK_2(x,xz) \in C^{(2)}[-1,1] \). Hence \( |\beta'_n(x)| \leq c_2 n^{-3/2} \). Similarly, \( |\beta''_n(x)| \leq c_1 n^{-1/2} \), providing the uniform convergence of all series involved in this section.

The validity of the formulas (6.11) and (6.12) in the general case can be verified by taking a sequence \( q_n \in C^2[0,b] \) such that \( q_n \to q \) uniformly as \( n \to \infty \), constructing corresponding integral kernels and coefficients \( \beta_n, \gamma_n \) for each \( q_n \) and passing to the limit in the formulas (6.11) and (6.12). The validity of Proposition 6.1 now follows by differentiating (6.11) and (6.12).

### 7 Numerical solution of spectral problems

The representations for solutions and their derivatives (4.1), (4.2) and (5.11), (5.12) lend themselves for numerical solving of equation (1.1) and in particular for numerical solving of related spectral problems. As an example, let us consider the Sturm-Liouville problem for (1.1),

\[
\begin{align*}
\alpha_0 y(0) + \mu_0 y'(0) &= 0, \\
\alpha_b y(b) + \mu_b y'(b) &= 0,
\end{align*}
\]

(7.1) where we allow the coefficients \( \alpha_0, \mu_0, \alpha_b \) and \( \mu_b \) to be not only constants but also entire functions of the square root \( \omega \) of the spectral parameter \( \lambda \) satisfying \( |\alpha_0| + |\mu_0| \neq 0 \) and \( |\alpha_b| + |\mu_b| \neq 0 \) (for every \( \lambda \)).

Based on the results of the previous sections and taking into account that the solutions \( c(\omega, x) \) and \( s(\omega, x) \) satisfy the following initial conditions

\[
\begin{align*}
c(\omega, 0) &= 1, & s(\omega, 0) &= 0, \\
c'(\omega, 0) &= h, & s'(\omega, 0) &= \omega,
\end{align*}
\]

we can formulate the following algorithm for solving spectral problems (7.1), (7.2) for equation (1.1).

1. Find a non-vanishing on \([0, b]\) solution \( f \) of the equation (2.1). Let \( f \) be normalized as \( f(0) = 1 \) and define \( h := f'(0) \). The solution \( f \) can be constructed using the SPPS representation, see, e.g., [26] for details or using any other numerical method.

2. Compute the functions \( \beta_k \) and \( \gamma_k \), \( k = 0, \ldots, N \) using (6.11) and (6.12).

3. Calculate the approximations \( c_N(\omega, x) \) and \( s_N(\omega, x) \) of the solutions \( c(\omega, x) \) and \( s(\omega, x) \) by (4.3) and (4.4). If necessary, calculate the approximations of the derivatives of the solutions using (5.13) and (5.14).

4. The eigenvalues of the problem (1.1), (7.1), (7.2) coincide with the squares of the zeros of the entire function

\[
\Phi(\omega) := \alpha_0 \left( \mu_0 c(\omega, b) - (\alpha_0 + \mu_0 h) \frac{s(\omega, b)}{\omega} \right) + \mu_b \left( \mu_0 c' (\omega, b) - (\alpha_0 + \mu_0 h) \frac{s'(\omega, b)}{\omega} \right)
\]

(7.3) and are approximated by squares of zeros of the function

\[
\Phi_N(\omega) := \alpha_0 \left( \mu_0 c_N(\omega, b) - (\alpha_0 + \mu_0 h) \frac{s_N(\omega, b)}{\omega} \right) + \mu_b \left( \mu_0 c' _N (\omega, b) - (\alpha_0 + \mu_0 h) \frac{s'_N(\omega, b)}{\omega} \right)
\]

(7.4)
5. The eigenfunction $y_\lambda$ corresponding to the eigenvalue $\lambda = \omega^2$ can be taken in the form

$$y_\lambda = \mu_0 c(\omega, x) - (\alpha_0 + \mu_0 h) \frac{s(\omega, x)}{\omega}.$$  

(7.5)

Hence once the eigenvalues are calculated the computation of the corresponding eigenfunctions can be done using formulas (4.3) and (4.4).

We have applied the proposed algorithm both in machine precision (in Matlab 2012) and in arbitrary precision arithmetics (in Mathematica 8.0). We refer the reader to [30, Section 7] for some implementation details concerning the computation of the system $\varphi_k$ and related numerical integration aspects. Though, as compared to [30], for the arbitrary precision arithmetics computation we used the modification of Clenshaw-Curtis integration method by Filippi [15] (see also [13, Section 6.4] and [44]) to calculate the functions $\varphi_k$, $\psi_k$, $\sigma_k$ and $\tau_k$. This method is reportedly more accurate for computing indefinite integrals, and we illustrate its performance in Example 7.2. Note that this method can be efficiently realized via Fast Fourier transform and for the improved accuracy the last coefficient $a_N$ in [13, (6.4.8) and (6.4.10)] has to be halved, c.f., [13, (2.13.1.10) and (2.13.1.11)]. For the machine precision calculations we used Newton-Cotes 6 point integration rule.

The independent evaluation of the spherical Bessel functions $j_k(\omega b)$ for all values of $k$ and all values of $\omega b$ using built-in routines from Matlab or Wolfram Mathematica can be rather slow. In order to speed up the evaluation of the series (4.3), (4.4), (5.13) and (5.14) the recurrent relations (6.2) can be used. We refer the reader to [3], [17] and references therein for further details.

Some numerical methods (such as Newton’s method) can benefit from the knowledge of the estimates of the partial sums can be obtained similarly to the previous sections.

Note that the coefficients $\{\beta_j\}$ and $\{\gamma_j\}$ as Fourier coefficients of smooth functions decrease to zero (not necessarily monotonically) as $j \to \infty$. The formulas presented in Definition 5.1 as well as (5.11) and (5.5) involve the dependence on all preceding functions and hence present computational difficulties due to the limited computation precision and cancelation of comparable terms. In Examples 7.2 [7.3] we illustrate this and show that the alternative formulas introduced in Section 8 allow one to compute more coefficients $\beta_k$ and $\gamma_k$. The following observation can be used to estimate an optimal number $N$ to choose.

**Remark 7.1.** The boundary conditions (5.11) offer a simple and efficient way for controlling the accuracy of the numerical method. Indeed, substitution of (5.2) into (5.1) leads to the equalities

$$\sum_{j=0}^{\infty} \frac{\beta_j(x)}{x} = \frac{h}{2} + \frac{1}{2} \int_0^x q(s) \, ds \quad \text{and} \quad \sum_{j=0}^{\infty} (-1)^j \frac{\beta_j(x)}{x} = \frac{h}{2}$$

(due to the relations $P_j(1) = 1$ and $P_j(-1) = (-1)^j$). The differences

$$\varepsilon_{1,N}(x) := \left| \sum_{j=0}^{N} \frac{\beta_j(x)}{x} - \left( \frac{h}{2} + \frac{1}{2} \int_0^x q(s) \, ds \right) \right| \quad \text{and} \quad \varepsilon_{2,N}(x) := \left| \sum_{j=0}^{N} (-1)^j \frac{\beta_j(x)}{x} - \frac{h}{2} \right|$$

(7.6)

indicate the accuracy of the approximation of the transmutation kernel and hence the accuracy of the approximate solutions (4.3) and (4.4).
Similarly, the accuracy of the coefficients $\gamma_k$ and the approximations (5.13) and (5.14) can be estimated using (5.4) and the following relations [31],

$$K_1(x, x) = \frac{1}{4} \left( q(x) + h \int_0^x q(s) \, ds + \frac{1}{2} \left( \int_0^x q(s) \, ds \right)^2 \right), \quad K_1(x, -x) = \frac{1}{4} \left( q(0) + \int_0^x q(s) \, ds \right).$$

The results of the previous section allow us to prove the uniform error bound for all approximate zeros of the characteristic function (at least when the coefficients in the boundary conditions (7.1) and (7.2) are independent of the spectral parameter) obtained by the proposed algorithm and that neither spurious zeros appear nor zeros are missed. For the proof we refer to [30, Section 7].

The proposed algorithm is based on the exact analytical representation of the solutions (4.1), (4.2) and their derivatives (5.11), (5.12). It can be easily combined with the widely used techniques such as the interval subdivision and the shooting method [39]. However we decided to perform the numerical experiments globally without any interval subdivision, to illustrate that even applied directly the algorithm provides accurate eigendata.

**Example 7.2.** Consider the following spectral problem (the first Paine problem, [36], see also [30, Example 7.4])

$$\begin{align*}
- u'' + e^x u &= \lambda u, \quad 0 \leq x \leq \pi, \\
u(0, \lambda) &= u(\pi, \lambda) = 0.
\end{align*}$$

![Figure 1: The plot of the absolute values of the coefficients $\beta_k(\pi)$, $k \leq 40$ from Example 7.2 (black line with asterisks) together with absolute errors obtained using formulas from Definition 3.1 (blue line with ‘x’ marks), formulas (3.1) (magenta line with ‘o’ marks) and formulas (6.11) (red line with ‘+’ marks).](image)

For the Matlab program we computed functions $\beta_k$, $k \leq 40$. All functions were represented by their values in 20001 uniformly spaced points. The modified Newton-Cotes 6 point integration rule was used to compute all integrals involved. In Mathematica we computed $\beta_k$ for $k \leq 200$ using 200 digit arithmetics and representing all functions by their 257 values at Tchebychev-spaced points, the Filippi modification of Clenshaw-Curtis formula was used for the numerical integration. As a particular solution we took $f(x) = I_0(2e^{x/2})$, however we did not use the explicit formula computing instead this particular solution numerically from the SPPS representation. Once again we would like to emphasize the excellent performance of the SPPS representation, the calculated particular solution coincided with the one provided by the exact formula up to Mathematica’s 200 digit accuracy.

On Figure 1 we present the absolute errors of the coefficients $\beta_k$ at $x = \pi$ computed in the machine precision using formulas from Definition 3.1 (3.1) and (6.11). As the exact values, the coefficients evaluated in Mathematica were used. As one can see, formula (6.11) performed much better, coefficient errors remain of essentially the same order while two other formulas produce exponential error growth.

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Figure 2: The plot of the maximum of the differences (7.6) at the point \( x = \pi \) from Example 7.2. The left graph corresponds to computation in the machine precision, the coefficients \( \beta_k, k \leq 40 \) obtained using formulas from Definition 5.1 (blue line with ‘x’ marks), formulas (3.1) (magenta line with ‘o’ marks) and formulas (6.11) (red line with ‘+’ marks). The right graph corresponds to computation in high precision arithmetics, the coefficients \( \beta_k, k \leq 200 \) obtained using formulas from Definition 5.1 (blue line with ‘x’ marks) and formulas (6.11) (magenta line with ‘+’ marks computed with the use of Clenshaw-Curtis integration method, red line with ‘+’ marks computed with Filippi’s modification).

As we mentioned before, formula (7.6) from Remark 7.1 can be used to estimate the number \( N \) of coefficients \( \beta_k \) computed correctly. On Figure 2 we present the maximum of two differences from (7.6) evaluated at \( x = \pi \) both in the machine precision and in the arbitrary precision arithmetics. The minimums on the first plot correlates with Figure 1. Again, a better performance of the formula (6.11) can be appreciated. For the arbitrary precision arithmetics, the minimum at \( N = 144 \) can be clearly seen and one can appreciate the better performance of the Filippi integration method in comparison with the Clenshaw-Curtis’ one. For the machine precision, the graph almost stabilizes at \( N = 29 \).

On Figure 3 we present the errors of the computed eigenvalues. For the machine precision we have taken \( N = 29 \) and \( N = 40 \) to illustrate that the proposed method is not sensible to the value of \( N \) while one chooses \( N \) from the stabilized part of the differences (7.6). As one can appreciate, the relative errors are close to the machine precision limit. For the arbitrary precision arithmetics we have taken \( N = 144 \) (an optimal number determined from Figure 2). As one can see, the eigenvalue errors remain uniformly bounded. The better precision of the first eigenvalues is explained by Proposition 4.4.

The computation time on a PC equipped with Intel i7-3770 microprocessor was: in machine precision – 0.25 seconds for constructing a particular solution and the coefficients \( \beta_k, k \leq 40 \) and 0.63 seconds for finding 500 eigenvalues with the help of secant method; in arbitrary precision arithmetics a particular solution and the coefficients \( \beta_k, k \leq 200 \) were computed in 9 seconds, 13 seconds more were necessary for our code based on Mathematica’s function FindRoot and recurrent relation (6.2) to find 500 eigenvalues. The maximum relative error of the first 500 eigenvalues computed in the machine precision was \( 2 \cdot 10^{-14} \), the maximum absolute error of the first 500 eigenvalues computed in the high precision was \( 6.3 \cdot 10^{-101} \).

Example 7.3. Consider the following spectral problem (the second Paine problem, [36], see also [30, Example 7.5])

\[
\begin{cases} 
-u'' + \frac{1}{(x+0.1)^2} u = \lambda u, & 0 \leq x \leq \pi, \\
 u(0, \lambda) = u(\pi, \lambda) = 0.
\end{cases}
\]

This problem was considered in [30, Example 7.5], where the results were reported for high precision arithmetics only. The reason was in the largeness of the coefficients arising in the solution of the approximation problem limiting the achievable accuracy of the approximation. As a result, the saturation occurred...
Figure 3: Errors of the first 200 eigenvalues from Example 7.2. Top plot: relative errors, obtained using machine precision and $N = 29$ (blue line with ‘x’ marks) and $N = 40$ (red line with ‘*’ marks). Bottom plot: absolute errors, obtained using high precision and $N = 144$.

Figure 4: The plot of the maximum of the differences (7.6) at the point $x = \pi$ from Example 7.3. The coefficients $\beta_k$, $k \leq 100$ obtained using formulas from Definition 3.1 (blue line with ‘x’ marks), formulas (3.1) (magenta line with ‘o’ marks) and formulas (6.11) (red line with ‘+’ marks).

starting from $N = 20$ and the eigenvalues were obtained with the error of about 0.001 or worse, see Figure 5.
The method proposed in this work allowed us to compute 84 coefficients $\beta_k$, see Figure 4, and 500 eigenvalues were calculated. On Figure 5 we present relative errors of the first 100 eigenvalues. The maximum relative error was $5.6 \cdot 10^{-15}$. The computation time was: 0.69 seconds for constructing a particular solution and the coefficients $\beta_k$, $k \leq 100$, and 0.8 seconds for finding 500 eigenvalues with the help of the secant method.

**Example 7.4.** Consider the following spectral problem (the truncated Gelfand-Levitan potential, [40])

$$-u'' + 2 \frac{T(x) \sin 2x + \cos^4 x}{T^2} u = \lambda u, \quad T(x) = 1 + \frac{x}{2} + \frac{\sin(2x)}{4}, \quad 0 \leq x \leq 100,$$

$$u(0, \lambda) - u'(0, \lambda) = u(100, \lambda) = 0.$$

The problem is considered difficult due to nonuniform oscillations of decreasing size in $q$.
calculate the coefficients $\beta_k$, $k \leq 160$. On Figure 5 (left plot) we present the maximum of the differences at $x = 100$. As one can see, the differences do not decrease until $N = 100$ and once again stabilize at $N = 144$. The formulas from Definition 3.1 do not serve to compute that large number of the coefficients in the machine precision, while formulas (6.11) provide such a possibility. We used $N = 144$ to compute the approximate eigenvalues. Since the exact eigenvalues of the problem are not known, we compared our results to the values reported in [40] as well as to those produced by the MATSLISE package [32]. In Table 1 we present several eigenvalues obtained. On Figure 5 (right plot) we show the differences between the eigenvalues computed by our method and by the MATSLISE package.

| $n$  | $\lambda_n$ (10) | $\lambda_n$ (our method) | $\lambda_n$ (MATSLISE) |
|------|------------------|----------------------------|------------------------|
| 0    | 0.00024681157    | 0.000246811787231069      | 0.000246811787231069   |
| 1    | 0.00222130735092850 | 0.00222130735093092     |
| 2    | 0.0061703052711158 | 0.0061703052711158      |
| 5    | 0.029864887478121 | 0.029864887478144        |
| 10   | 0.108847814083180 | 0.108847814083183       |
| 20   | 0.414974806699760 | 0.414974806699766        |
| 50   | 2.51650713279491  | 2.51650713279492         |
| 99   | 9.770828528216    | 9.77082852802586         | 9.77082852802587       |

Table 1: Eigenvalues from Example 7.4

Example 7.5. Consider the following problem with spectral parameter depending boundary conditions

$$\begin{align*}
-u'' + Q(x)u &= \lambda u, \quad x \in [0, 2a], \\
u'(0) - \nu u(0) &= 0, \\
u'(2a) + \nu u(2a) &= 0,
\end{align*}$$

where $\lambda = -\nu^2$ and $Q(x) = -m(m+1) \sech^2(x-a)$, $m \in \mathbb{N}$. This spectral problem arises in relation with quantum wells when the sech-squared potential $q(x) = -m(m+1) \sech^2 x$, $x \in (-\infty, \infty)$ is truncated, see [10] and [30, Sect. 7.4] for details. As was mentioned in [30, Sect. 7.4], the physically meaningful region for the eigenvalues of a quantum well problem is $\lambda \in [\min_{x \in [0,2a]} Q(x), 0]$ and in the particular case under consideration, the non-truncated problem possesses exactly $m$ eigenvalues given by $\lambda_n = -(m-n)^2$, $n = 0, 1, \ldots, m-1$. In the notations of this work we have $\omega = i\nu$, the region to look for the eigenvalues is $\nu \in (0, \sqrt{m(m+1)})$ and the characteristic function (7.3) can be written in the form

$$c'(\omega, 2a) - \frac{(i\omega + h)}{w} s'(\omega, 2a) - i\omega c(\omega, 2a) + i(i\omega + h)s(\omega, 2a).$$

For the numerical experiment we chose $a = 8$ and $m = 3$ and 5. All calculations were performed in Matlab in the machine precision. 50001 points (for $m = 3$) and 80001 points (for $m = 5$) were used to represent all the functions involved, and the alternative formulas (6.11) and (6.12) were used to compute the coefficients $\beta_k$ and $\gamma_k$. For $m = 3$ the optimal $N$ was found to be 51, while for $m = 5$ the optimal $N$ was 63. The computed eigenvalues are presented in Table 2.

| $n$  | Exact $\lambda_n$ | $\lambda_n$ (our method) | $\lambda_n$ (10) |
|------|-------------------|--------------------------|------------------|
| 0    | -9                | -9.00000001319           | -8.999628656     |
| 1    | -4                | -3.99999999103           | -3.999998053     |
| 2    | -1                | -1.00000000089           | -0.999927816     |

| $n$  | Exact $\lambda_n$ | $\lambda_n$ (our method) |
|------|-------------------|--------------------------|
| 0    | -25               | -25.00003450              |
| 1    | -16               | -15.99994465              |
| 2    | -9                | -9.000027727              |
| 3    | -4                | -3.99995313               |
| 4    | -1                | -1.00000082               |

Table 2: Approximations of $\lambda_n$ of the potential $-m(m+1) \sech^2 x$ (Example 7.5) for $m = 3$ and $m = 5.$
Example 7.6. Consider the following spectral problem with a complex valued potential \([5]\),
\[
\begin{cases}
-u'' + (1 + i)x^2 u = \lambda u, & 0 \leq x \leq \pi, \\
u(0, \lambda) = u(\pi, \lambda) = 0.
\end{cases}
\]

We computed 40 eigenvalues of this problem in Matlab in the machine precision. All the functions involved were represented by their values in 4001 points. Alternative formulas for the coefficients \(\beta_k\) were used and \(N = 27\) was find to be optimal for the machine precision arithmetics. The eigenvalues of the problem are complex numbers and they were localized using the argument principle, see \([24, \text{Example 5.6}]\) for further details. After the zeros were localized within rectangles with the sides smaller than \(0.1\), we applied several Newton iterations to obtain approximate eigenvalues. On Figure 7 we illustrate the work of the algorithm based on the argument principle. The approximate eigenvalues were compared with the values obtained from the exact characteristic equation using Wolfram Mathematica. We present several eigenvalues in Table 3. The relative errors of the obtained eigenvalues were less than \(9.5 \cdot 10^{-15}\), while the relative errors of the eigenvalues reported in \([5]\) were between \(4.9 \cdot 10^{-6}\) and \(5.8 \cdot 10^{-4}\). Moreover, the absolute error of the 40th eigenvalue was \(2 \times 10^{-12}\) (our method) compared to 0.94 \([5]\).

| \(n\) | \(\lambda_n \text{ (Exact)}\) | \(\lambda_n \text{ (our method)}\) | \(\lambda_n \text{ ([5])}\) |
|-------|-----------------|-----------------|-----------------|
| 1     | 3.29252447095779 + 1.36633744750457i | 3.29252447095781 + 1.36633744750457i | 3.292530 + 1.366321i |
| 2     | 7.55904717588808 + 3.05068659781596i | 7.55904717588808 + 3.05068659781596i | 7.559344 + 3.050606i |
| 3     | 12.33983661951932 + 3.59139777785523i | 12.33983661951938 + 3.59139777785521i | 12.34084 + 3.59194i |
| 5     | 28.26784723460268 + 3.43290953376002i | 28.26784723460276 + 3.43290953376002i | 28.26883 + 3.43560i |
| 10    | 103.2845071723909 + 3.3276829117743i | 103.2845071723903 + 3.3276829117725i | 103.2855 + 3.3390i |
| 20    | 403.2885939386633 + 3.2994114805675i | 403.2885939386637 + 3.2994114805679i | 403.2893 + 3.3512i |
| 40    | 1603.289554053531 + 3.29225803189i | 1603.289554053531 + 3.29225803189i | 1603.139 + 4.214i |

Table 3: Eigenvalues from Example 7.6.

8 Conclusions

The representations \([4.1], [4.2]\) of solutions to \([1.1]\) are proved together with the representations \([5.11], [5.12]\) of their derivatives. For the coefficients \(\beta_k\) and \(\gamma_k\) in \([1.1], [4.2], [5.11]\) and \([5.12]\) besides the closed form formulas \([3.1], [5.6]\) a recurrent integration procedure is developed. Estimates, uniform with respect to \(\omega\), for the rate of convergence of the series involved in the representations are obtained. It is shown that besides offering new analytical representations of solutions, formulas \([4.1], [4.2], [5.11]\) and \([5.12]\) put at
one’s disposal a simple and powerful numerical method for solving initial value and spectral problems for (1.1). Due to the uniformity of the approximation with respect to $\omega$, the numerical method based on (4.1), (4.2), (5.11) and (5.12) allows one to compute within seconds large sets of eigendata with a nondeteriorating accuracy.

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