A Neumann series of Bessel functions representation for solutions of Sturm-Liouville equations

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Abstract

A Neumann series of Bessel functions (NSBF) representation for solutions of Sturm-Liouville equations and for their derivatives is obtained. The representation possesses an attractive feature for applications: for all real values of the spectral parameter \( \omega \) the difference between the exact solution and the approximate one (the truncated NSBF) depends on \( N \) (the truncation parameter) and the coefficients of the equation and does not depend on \( \omega \). A similar result is valid when \( \omega \in \mathbb{C} \) belongs to a strip \(|\text{Im} \omega| < C\). This feature makes the NSBF representation especially useful for applications requiring computation of solutions for large intervals of \( \omega \). Error and decay rate estimates are obtained. An algorithm for solving initial value, boundary value or spectral problems for the Sturm-Liouville equation is developed and illustrated on a test problem.

1 Introduction

In the recent work [13] a new representation for solutions of the one-dimensional Schrödinger equation

\[
-u'' + Q(x)u = \omega^2 u
\]

was obtained in terms of so-called (see, e.g., [24], [25] and [2]) Neumann series of Bessel functions (NSBF). The representation possesses an attractive feature for applications: for all \( \omega \in \mathbb{R} \) the difference between the exact solution and the approximate one (the truncated NSBF) depends on \( N \) (the truncation parameter) and \( Q \) and does not depend on \( \omega \). A similar result is valid when \( \omega \in \mathbb{C} \) belongs to a strip \(|\text{Im} \omega| < C\). This feature makes the NSBF representation especially useful for applications requiring computation of solutions for large intervals of \( \omega \). For example, as was shown in [13], the NSBF representation allows one to compute hundreds or if necessary even thousands of eigendata with a nondeteriorating for large \( \omega \) and remarkable accuracy. In [15] the NSBF representation was extended onto perturbed Bessel equations.

In the present work we derive an NSBF representation for solutions of the Sturm-Liouville equation

\[
-(p(y)v')' + q(y)v = \omega^2 r(y)v.
\]

The coefficients are assumed to admit the application of the Liouville transformation (see, e.g., [6], [26]). The main result consists in an NSBF representation for solutions of (1.2) and for their

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derivatives, preserving the same attractive feature described above. Error and decay rate estimates are obtained. An algorithm for solving initial value, boundary value or spectral problems for (1.2) is developed and illustrated on a test problem.

Besides this Introduction the paper contains the following sections. Section 2 presents some well known facts concerning the Liouville transformation together with recent results from [11] showing how the system of formal powers associated with (1.2) is transformed by the Liouville transformation. In Section 3 we recall some relevant results from [13] which are used in Section 4 and Section 5 for obtaining the main results of this work, the NSBF representation for solutions of (1.2) as well as for their derivatives. In Section 6 convenient for computation formulas for the coefficients of the NSBF representations are derived. In Section 7 a computational algorithm based on the NSBF representation is formulated and discussed. Section 8 presents some illustrations of its numerical performance on a test problem admitting an exact solution. In Appendix A we prove error and decay rate estimates of the NSBF representation.

2 Preliminaries on the Liouville transformation

2.1 Definition of the Liouville transformation

Consider the Sturm-Liouville differential equation

\[(p(y)v')' - q(y)v = -\lambda r(y)v, \quad y \in [A,B],\]  \hspace{1cm} (2.1)

with \([A,B]\) being a finite interval. Let \(q : [A,B] \to \mathbb{C}, \) \(p \) and \(r : [A,B] \to \mathbb{R}\) be such that \(q \in C[A,B], p, p', r, r' \in AC[A,B]\) and \(p(y) > 0, r(y) > 0\) for all \(y \in [A,B].\) Define the mapping \(l : [A,B] \to [0,b]\) by

\[l(y) := \int_{A}^{y} \frac{r(s)/p(s)}{\rho(s)} \frac{1}{2} ds, \]  \hspace{1cm} (2.2)

where \(b = \int_{A}^{B} \frac{r(s)/p(s)}{\rho(s)} \frac{1}{2} ds.\) Denote \(\rho(y) := (p(y)r(y))^{1/4}.\) Then (2.1) is related to the one-dimensional Schrödinger differential equation

\[u'' - Q(x)u = -\lambda u, \quad x \in [0,b]\]  \hspace{1cm} (2.3)

by the Liouville transformation of the variables \(y\) and \(v\) into \(x\) and \(u\) defined as (see, e.g., [6], [26])

\[x = l(y), \quad u(x) := \rho(y)v(y) \quad \text{for all } y \in [A,B]\]

and the coefficient \(Q\) is given by the relation

\[Q(x) = \frac{q(y)}{r(y)} + \frac{p(y)}{4r(y)} \left[ \left( \frac{p'(y)}{p(y)} + \frac{r'(y)}{r(y)} \right) + \frac{3}{4} \left( \frac{p'(y)}{p(y)} \right)^2 + \frac{1}{2} \frac{p'(y)r'(y)}{p(y)r(y)} - \frac{1}{4} \left( \frac{r'(y)}{r(y)} \right)^2 \right] \]  \hspace{1cm} (2.4)

and

\[\frac{q(y)}{r(y)} - \frac{\rho(y)}{r(y)} \left[ p(y) \left( \frac{1}{\rho(y)} \right) \right]' \quad \text{for all } y \in [A,B].\]

The Liouville transformation can be considered as an operator \(L : C[A,B] \to C[0,b]\) acting according to the rule

\[u(x) = L[v(y)] = \rho(l^{-1}(x))v(l^{-1}(x)).\]

Let us introduce the following notations for the differential expressions

\[B = -\frac{d^2}{dx^2} + Q(x) \quad \text{and} \quad C = -\frac{1}{r(y)} \left( \frac{d}{dy} \left( p(y) \frac{d}{dy} \right) - q(y) \right).\]

The following proposition summarizes the main properties of the operator \(L.\)
Remark 2.3.  The formal powers arise in the spectral parameter power series (SPPS) representation of solutions of equation (2.3).

Proposition 2.1.  
1. The inverse operator is defined by $v(y) = L^{-1}[u(x)] = \frac{1}{\rho(y)} u(l(y))$.

2. The uniform norms of the operators $L$ and $L^{-1}$ are $\|L\| = \max_{y \in [A, B]} |\rho(y)|$ and $\|L^{-1}\| = \max_{y \in [A, B]} |1/\rho(y)|$.

3. The operator equality

$$BL = LC$$

is valid on $C^2(A, B) \cap C[A, B]$.

2.2 Transformation of formal powers

Let $f$ be a non-vanishing solution of the equation

$$f'' - Q(x)f = 0, \quad x \in [0, b],$$

such that

$$f(0) = 1.$$  

On the existence of a non-vanishing $f$ see Remark 2.5 below. Note that in general complex valued solutions are considered even when the coefficient $Q$ is real valued. Denote $h := f'(0) \in \mathbb{C}$.

Consider two sequences of recursive integrals (see [10], [12], [14])

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

and

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

Definition 2.2. The families of functions $\{\varphi_k\}_{k=0}^\infty$ and $\{\psi_k\}_{k=0}^\infty$ constructed according to the rules

$$\varphi_k(x) = \begin{cases} f(x)X^{(k)}(x), & k \text{ odd}, \\ f(x)\bar{X}^{(k)}(x), & k \text{ even} \end{cases} \quad \text{and} \quad \psi_k(x) = \begin{cases} X^{(k)}(x), & k \text{ odd}, \\ f(x)X^{(k)}(x), & k \text{ even} \end{cases}$$

are called systems of formal powers associated with equation (2.3).

Remark 2.3. The formal powers arise in the spectral parameter power series (SPPS) representation for solutions of (2.3) (see [9], [10], [12], [14]).

Analogously, let us introduce a system of formal powers corresponding to equation (2.1).

Let $g$ be a solution of the equation

$$(p(y)g')' - q(y)g = 0, \quad y \in [A, B],$$

such that $g(y) \neq 0$ for all $y \in [A, B]$ (see Remark 2.5). Then the following two families of auxiliary functions are well defined

$$\bar{Y}^{(0)}(y) \equiv Y^{(0)}(y) \equiv 1,$$

$$Y^{(n)}(y) = \begin{cases} n \int_A^y Y^{(n-1)}(s) \frac{1}{g^2(s)\rho(s)} ds, & n \text{ odd}, \\ n \int_A^y Y^{(n-1)}(s)g^2(s)r(s) ds, & n \text{ even}, \end{cases}$$

$$\bar{Y}^{(n)}(y) = \begin{cases} n \int_A^y \bar{Y}^{(n-1)}(s) \frac{1}{g^2(s)\rho(s)} ds, & n \text{ odd}, \\ n \int_A^y \bar{Y}^{(n-1)}(s)g^2(s)r(s) ds, & n \text{ even}. \end{cases}$$

Then similarly to Definition 2.2 we define the formal powers associated to equation (2.1).
Definition 2.4. Let \( p, q, r \) satisfy conditions of Subsection 2.1 and \( g \) be a non-vanishing solution of (2.6). Then the formal powers associated to equation (2.1) are defined for any \( k \in \mathbb{N} \cup \{0\} \) as follows

\[
\Phi_k(y) = \begin{cases} 
  g(y)Y^{(k)}(y), & k \text{ odd}, \\
  g(y)\tilde{Y}^{(k)}(y), & k \text{ even}, 
\end{cases}
\]

and

\[
\Psi_k(y) = \begin{cases} 
  \frac{1}{g(y)}Y^{(k)}(y), & k \text{ even}, \\
  \frac{1}{g(y)}\tilde{Y}^{(k)}(y), & k \text{ odd}.
\end{cases}
\]

Remark 2.5. The existence of a non-vanishing solution of (2.6) for complex valued \( p \) and \( q \) such that \( p, p' \) and \( q \) are continuous on \([A, B]\) was proved in [14, Remark 5] (see also [7]). Moreover, the only reason for the requirement of the absence of zeros of the functions \( f \) and \( g \) is to make sure that the formal powers be well defined. As was shown in [16] this is true even when \( f \) and/or \( g \) have zeros, though in that case corresponding formulas are slightly more complicated.

Theorem 2.6 ([11]). Let \( p, q, r \) and \( g \) be functions satisfying the conditions of Definition 2.4, and hence \( f(x) = f(l(y)) := \rho(y)g(y) \) is a particular solution of \((2.5)\). Then the following relations are valid

\[
\rho(y)\Phi_n(y) = \varphi_n(x) \quad \text{and} \quad \frac{1}{\rho(y)}\Psi_n(y) = \psi_n(x) \quad \text{for all } n \in \mathbb{N} \cup \{0\},
\]

that is

\[
\varphi_n(x) = L[\Phi_n(y)] \quad \text{and} \quad \psi_n(x) = L[\Psi_n(y)/\rho^2(y)].
\]

In order that the equality \( f(0) = 1 \) be fulfilled, \( g \) must be chosen so that

\[
g(A) = \frac{1}{\rho(A)}. \tag{2.7}
\]

We will assume this initial condition to be satisfied.

It is easy to see that for \( h = f'(0) \) one obtains

\[
h = \sqrt{\frac{p(A)}{r(A)} \left( \frac{g'(A)}{g(A)} + \frac{\rho'(A)}{\rho(A)} \right)}. \tag{2.8}
\]

3 Solution of the one-dimensional Schrödinger equation

Let \( \omega = \sqrt{\lambda} \), and \( c(\omega, x), s(\omega, x) \) denote the solutions of (2.3) satisfying the following initial conditions in the origin

\[
c(\omega, 0) = 1, \quad c'(\omega, 0) = h, \quad s(\omega, 0) = 0, \quad s'(\omega, 0) = \omega \tag{3.1}
\]

where \( h \) is an arbitrary complex number.

Theorem 3.1 ([13]). The solutions \( c(\omega, x) \) and \( s(\omega, x) \) of the equation

\[
u'' - Q(x)u = -\omega^2 u, \quad x \in (0, b)
\]

admit the following representations

\[
c(\omega, x) = \cos \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n}(x)j_{2n}(\omega x) \tag{3.2}
\]

and

\[
s(\omega, x) = \sin \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n+1}(x)j_{2n+1}(\omega x) \tag{3.3}
\]
where \( j_k \) stands for the spherical Bessel function of order \( k \), the functions \( \beta_n \) are defined as follows

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

where \( l_{k,n} \) is the coefficient of \( x^k \) in the Legendre polynomial of order \( n \). The series in (3.2) and (3.3) 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

\[
c_N(\omega, x) = \cos \omega x + 2 \sum_{n=0}^{\lfloor N/2 \rfloor} (-1)^n \beta_{2n}(x) j_{2n}(\omega x) \quad (3.5)
\]

and

\[
s_N(\omega, x) = \sin \omega x + 2 \sum_{n=0}^{\lfloor (N-1)/2 \rfloor} (-1)^n \beta_{2n+1}(x) j_{2n+1}(\omega x) \quad (3.6)
\]

the following uniform estimates hold

\[
|c(\omega, x) - c_N(\omega, x)| \leq \sqrt{2x} \varepsilon_N(x) \quad \text{and} \quad |s(\omega, x) - s_N(\omega, x)| \leq \sqrt{2x} \varepsilon_N(x) \quad (3.7)
\]

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

\[
|c(\omega, x) - c_N(\omega, x)| \leq \varepsilon_N(x) \frac{\sinh(2Cx)}{C} \quad \text{and} \quad |s(\omega, x) - s_N(\omega, x)| \leq \varepsilon_N(x) \frac{\sinh(2Cx)}{C} \quad (3.8)
\]

for any \( \omega \in \mathbb{C}, \omega \neq 0 \) belonging to the strip \( |\text{Im} \omega| \leq C, C \geq 0 \). Here \( \varepsilon_N \) is a function satisfying \( \varepsilon_N \to 0 \) as \( N \to \infty \). These estimates are slight refinements for those presented in [13], using the ideas from [15]. Some estimates for \( \varepsilon_N(x) \) are presented in Appendix A.

Inequalities (3.7) and (3.8) reveal an interesting feature of the representations (3.2) and (3.3): the accuracy of approximation of the exact solutions by the partial sums (3.5) and (3.6) does not depend on \( \omega \) meanwhile it belongs to a strip \( |\text{Im} \omega| \leq C \) in the complex plane. This feature was tested and confirmed numerically in [13]. An analogous result is valid for the derivatives of the solutions. We formulate it in the following statement.

**Theorem 3.2 ([13]).** The derivatives of the solutions \( c(\omega, x) \) and \( s(\omega, x) \) with respect to \( x \) admit the following representations

\[
c'(\omega, x) = -\omega \sin \omega x + \left( h + \frac{1}{2} \int_0^x Q(s) \, ds \right) \cos \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \gamma_{2n}(x) j_{2n}(\omega x) \quad (3.9)
\]

and

\[
s'(\omega, x) = \omega \cos \omega x + \frac{1}{2} \left( \int_0^x Q(s) \, ds \right) \sin \omega x + 2 \sum_{n=0}^{\infty} (-1)^n \gamma_{2n+1}(x) j_{2n+1}(\omega x) \quad (3.10)
\]

where \( \gamma_n \) are defined as follows

\[
\gamma_n(x) = \frac{2n+1}{2} \left( \sum_{k=0}^{n} l_{k,n} \left( \frac{k \psi_{k-1}(x)}{f(x)} + \frac{r(x)}{f(x)} \right) - \frac{n(n+1)}{2x} - \frac{1}{2} \int_0^x Q(s) \, ds - \frac{h}{2} (1 + (-1)^n) \right). \quad (3.11)
\]
The series in (3.9) and (3.10) 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 approximations
\[
c_\omega(x) := -(\omega \sin x + \left(h + \frac{1}{2}\right) \int_0^x Q(s) \, ds) \cos x + 2 \sum_{n=0}^{[N/2]} (-1)^n \gamma_{2n}(x) j_{2n}(\omega x)
\]
and
\[
s_\omega(x) := \omega \cos x + \frac{1}{2} \left( \int_0^x Q(s) \, ds \right) \sin x + 2 \sum_{n=0}^{[N-1/2]} (-1)^n \gamma_{2n+1}(x) j_{2n+1}(\omega x)
\]
the following inequalities are valid
\[
\left| c'(\omega, x) - c_\omega(x) \right| \leq \sqrt{2x \epsilon_{1,N}(x)} \quad \text{and} \quad \left| s'(\omega, x) - s_\omega(x) \right| \leq \sqrt{2x \epsilon_{1,N}(x)}
\]
for any $\omega \in \mathbb{R}$, $\omega \neq 0$, and
\[
\left| c'(\omega, x) - c_\omega(x) \right| \leq \epsilon_{1,N}(x) \frac{\sinh(2C \epsilon)}{C} \quad \text{and} \quad \left| s'(\omega, x) - s_\omega(x) \right| \leq \epsilon_{1,N}(x) \frac{\sinh(2C \epsilon)}{C}
\]
for any $\omega \in \mathbb{C}$, $\omega \neq 0$ belonging to the strip $|\text{Im}\, \omega| \leq C$, $C \geq 0$.

**Remark 3.3** (13). The functions $\beta_n$ also can be constructed as solutions of the recurrent equations
\[
\frac{1}{x^{n}} \mathbf{B}[x^{n} \beta_{n}(x)] = \frac{2n + 1}{2n - 3} x^{n-1} \mathbf{B}\left[ \frac{\beta_{n-2}(x)}{x^{n-1}} \right], \quad n \geq 1,
\]
with the first functions given by $\beta_{-1} := 1/2$ and $\beta_{0} = (f - 1)/2$ and initial conditions $\sigma_{n}(0) = \sigma'_{n}(0) = 0$ where $\sigma_{n}(x) := x^{n} \beta_{n}(x)$.

The functions $\gamma_n$ can be calculated from the equalities
\[
\gamma_{-1}(x) = \frac{1}{4} \int_0^x Q(s) \, ds,
\]
\[
\gamma_{0}(x) = \beta'_{0}(x) - \frac{h}{2} - \frac{1}{4} \int_0^x Q(s) \, ds = \frac{f'(x)}{2} - \frac{h}{2} - \frac{1}{4} \int_0^x Q(s) \, ds,
\]
\[
\gamma_{n}(x) = \frac{n}{x} \beta_{n}(x) + \beta'_{n}(x) + \frac{2n + 1}{2n - 3} \left( \gamma_{n-2}(x) - \beta_{n-2}(x) + \frac{n-1}{x} \beta_{n-2}(x) \right), \quad n \geq 1.
\]
One can use $\gamma_{1}(x) = \frac{1}{x} \beta_{1}(x) + \beta'_{1}(x) - \frac{3}{4} \int_0^x Q(s) \, ds$ as well.

**Remark 3.4.** Based on the formulas from Remark 3.3 a stable recurrent integration procedure for computing the functions $\sigma_n$ and $\tau_n := x^n \gamma_n$ was proposed in [13] in the following form.

\[
\eta_{n}(x) = \int_0^x \left( tf'(t) + (n-1)f(t) \right) \sigma_{n-2}(t) \, dt, \quad \theta_{n}(x) = \int_0^x \frac{1}{f^2(t)} \left( \eta_{n}(t) - tf(t) \sigma_{n-2}(t) \right) \, dt,
\]
\[
\sigma_{n}(x) = \frac{2n + 1}{2n - 3} \left[ x^2 \sigma_{n-2}(x) + c_{n} f(x) \theta_n(x) \right],
\]
\[
\tau_{n}(x) = \frac{2n + 1}{2n - 3} \left[ x^2 \tau_{n-2}(x) + c_{n} \left( f'(x) \theta_{n}(x) + \frac{\eta_{n}(x)}{f(x)} \right) - (c_{n} - 2n + 1)x \sigma_{n-2}(x) \right], \quad n \geq 1,
\]
where $c_{n} = 1$ if $n = 1$ and $c_{n} = 2(2n - 1)$ otherwise.
4 Solution of the Sturm-Liouville equation

Let us generalize Theorems 3.1 and 3.2 onto solutions of equation (2.1).

**Theorem 4.1.** Let the functions $p, q$ and $r$ satisfy the conditions from Subsection 2.1 and $g$ be a solution of (2.6) satisfying (2.7) and such that $g(y) \neq 0$ for all $y \in [A, B]$. Then two linearly independent solutions $v_1$ and $v_2$ of equation (2.1) for $\omega \neq 0$ can be written in the form

\[
v_1(\omega, y) = \cos \left( \frac{\omega l(y)}{\rho(y)} \right) + 2 \sum_{n=0}^{\infty} (-1)^n \alpha_{2n}(y) j_{2n}(\omega l(y))
\]

and

\[
v_2(\omega, y) = \sin \left( \frac{\omega l(y)}{\rho(y)} \right) + 2 \sum_{n=0}^{\infty} (-1)^n \alpha_{2n+1}(y) j_{2n+1}(\omega l(y))
\]

with $l(y)$ defined by (2.2), the coefficients $\alpha_n$ being defined by the equalities

\[
\alpha_n(y) = \frac{2n + 1}{2} \left( \sum_{k=0}^{n} \frac{l_{k,n} \Phi_k(y)}{l^k(y)} - \frac{1}{\rho(y)} \right),
\]

where $\Phi_k$ are from Definition 2.4. The solutions $v_1$ and $v_2$ satisfy the following initial conditions

\[
v_1(\omega, A) = \frac{1}{\rho(A)}, \quad v_2(\omega, A) = 0,
\]

\[
v_1'(\omega, A) = g'(A), \quad v_2'(\omega, A) = \frac{\omega}{\rho(A)} \sqrt{\frac{r(A)}{p(A)}}.
\]

The series in (4.1) and (4.2) converge uniformly with respect to $y$ on $[A, B]$ and converge uniformly with respect to $\omega$ on any compact subset of the complex plane of the variable $\omega$.

Moreover, for the functions

\[
v_1^N(\omega, y) = \cos \left( \frac{\omega l(y)}{\rho(y)} \right) + 2 \sum_{n=0}^{\left[ N/2 \right]} (-1)^n \alpha_{2n}(y) j_{2n}(\omega l(y))
\]

and

\[
v_2^N(\omega, y) = \sin \left( \frac{\omega l(y)}{\rho(y)} \right) + 2 \sum_{n=0}^{\left[ (N-1)/2 \right]} (-1)^n \alpha_{2n+1}(y) j_{2n+1}(\omega l(y))
\]

the following estimates hold

\[
|v_{1,2}(\omega, y) - v_{1,2}^N(\omega, y)| \leq 2(l(y)\varepsilon_N(l(y))) \max_{y \in [A,B]} \frac{1}{\rho(y)}
\]

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

\[
|v_{1,2}(\omega, y) - v_{1,2}^N(\omega, y)| \leq \varepsilon_N(l(y)) \sqrt{\frac{\sinh(2C l(y))}{C}} \max_{y \in [A,B]} \frac{1}{\rho(y)}
\]

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 function from Theorem 3.1.
Proof. Consider solutions (3.2) and (3.3) of (2.3). The functions

\[ v_1(\omega, y) = \mathbb{L}^{-1} [c(\omega, x)] = \frac{1}{\rho(y)} \left( \cos(\omega l(y)) + 2 \sum_{n=0}^{\infty} (-1)^n \beta_2 n(l(y)) j_{2n}(\omega l(y)) \right) \]

and

\[ v_2(\omega, y) = \mathbb{L}^{-1} [s(\omega, x)] = \frac{1}{\rho(y)} \left( \sin(\omega l(y)) + 2 \sum_{n=0}^{\infty} (-1)^n \beta_{2n+1}(l(y)) j_{2n+1}(\omega l(y)) \right) \]

are then solutions of (2.1) with \( \omega \) obtained by applying Remark 4.2. Inequalities (4.3) and thus the solutions (4.4) follow from (3.1). Indeed, due to statement 1. from Proposition 2.1, \( v(x) \) and any \( \frac{\rho v}{\omega} \) of the Liouville transformation we have the equality (4.4) and (4.5). From the definition of the Liouville transformation we have the equality \( \langle \rho v \rangle = u_x \rho_y \) for any function \( u \) and \( v \) being related by \( u(x) = \mathbb{L}[v(y)] \), and thus,

\[ v_y = \frac{1}{\rho} \left( \sqrt{\frac{\tau}{p}} u_x - \rho_y v \right), \tag{4.11} \]

from where (4.5) are derived.

\[ \Box \]

Remark 4.2. Inequalities (4.8) and (4.9) show that the representations (4.1) and (4.2) preserve the important property of the representations (3.2) and (3.3): the accuracy of approximation of the exact solutions by the partial sums (4.9) and (4.10) does not depend on \( \omega \) meanwhile it belongs to a strip \( \text{Im} \omega \leq C \) in the complex plane.

Remark 4.3. Similarly to the coefficients \( \beta_n \) (see Remark 3.3) the functions \( \alpha_n \) can be constructed as solutions of the recurrent equations

\[ \frac{1}{ln(y)} C [n(y) \alpha_n(y)] = \frac{2n + 1}{2n - 3} l^{n-1}(y) C \left[ \frac{\alpha_{n-2}(y)}{l^{n-1}(y)} \right] \tag{4.12} \]

obtained by applying \( \mathbb{L}^{-1} \) to (3.12) and taking into account (4.10) and the equality \( \mathbb{L}^{-1} B = C \mathbb{L}^{-1} \). The first functions of the sequence \( \{\alpha_n\} \) are given by

\[ \alpha_{-1} = \mathbb{L}^{-1} [\beta_{-1}] = \frac{1}{2 \rho} \quad \text{and} \quad \alpha_0 = \mathbb{L}^{-1} [\beta_0] = \frac{1}{2} \left( g - \frac{1}{\rho} \right). \tag{4.13} \]
The initial conditions satisfied by $\Sigma_n(y) := l^n(y)\alpha_n(y)$ have the form

$$
\Sigma_n(A) = \Sigma_n'(A) = 0.
$$

This sequence of equations for $\{\alpha_n\}$ leads to a stable recursive integration procedure which is proposed in Section 6.

### 5 Representation of the derivatives of the solutions $v_1$ and $v_2$

Due to (4.11) for $v_1(\omega, y) = L^{-1} [c(\omega, x)]$ and $v_2(\omega, y) = L^{-1} [s(\omega, x)]$ with the aid of (3.9), (3.10) and (4.1), (4.2) we obtain

$$
v'_1(\omega, y) = \sqrt{r(y)} \left( \frac{1}{\rho(y)} (G_1(y) \cos(\omega l(y)) - \omega \sin(\omega l(y))) + \sum_{n=0}^{\infty} (-1)^n \mu_{2n}(y) j_{2n}(\omega l(y)) \right)
- \frac{\rho'(y)}{\rho(y)} v_1(\omega, y)
$$

(5.1)

and

$$
v'_2(\omega, y) = \sqrt{r(y)} \left( \frac{1}{\rho(y)} (G_2(y) \sin(\omega l(y)) + \omega \cos(\omega l(y))) + \sum_{n=0}^{\infty} (-1)^n \mu_{2n+1}(y) j_{2n+1}(\omega l(y)) \right)
- \frac{\rho'(y)}{\rho(y)} v_2(\omega, y)
$$

(5.2)

where

$$
\mu_n(y) := \frac{\gamma_n(l(y))}{\rho(y)} = L^{-1} [\gamma_n(x)], \quad n = 0, 1, 2, \ldots,
$$

and the functions $G_1$ and $G_2$ have the form (cf. [11, Remark 4.7])

$$
G_1(y) := h + \frac{1}{2} \int_0^{r(y)} Q(s) \, ds = h + \frac{1}{2} \int_A^{y} \frac{1}{(pr)^{1/4}} \left( \frac{q}{(pr)^{1/4}} - [p((pr)^{-1/4})'] \right) (s) \, ds
$$

$$
= h + \frac{\rho'}{2r} \left|_A^y \right. + \frac{1}{2} \int_A^y \left[ \frac{q}{\rho^2} + \frac{\rho'^2}{r} \right] (s) \, ds
$$

(5.3)

and

$$
G_2(y) := \frac{1}{2} \int_0^{l(y)} Q(s) \, ds = G_1(y) - h.
$$

(5.4)

Let us obtain a formula for calculating $\mu_n$ which would not involve magnitudes related to equation (2.3) but only those related to (2.1). Consider (3.11). Direct calculation gives us the relation

$$
\frac{f'(x)}{f(x)} = \sqrt{\frac{p(y)}{r(y)} \left( \frac{g'(y)}{g(y)} + \frac{\rho'(y)}{\rho(y)} \right)}.
$$

Hence, due to Theorem 2.6

$$
k\psi_{k-1}(x) + f'(x)\varphi_k(x)/f(x) = k\frac{\Psi_{k-1}(y)}{\rho(y)} + \rho(y) \sqrt{\frac{p(y)}{r(y)} \left( \frac{g'(y)}{g(y)} + \frac{\rho'(y)}{\rho(y)} \right)} \Phi_k(y).
$$
Thus,
\[ \mu_n(y) = \frac{2n+1}{2\rho(y)} \left( \sum_{k=0}^{n} \frac{l_{k,n}(y)}{k!} \left( k \frac{\Psi_{k-1}(y)}{\rho(y)} + \rho(y) \sqrt{\frac{p(y)}{r(y)}} \left( \frac{g'(y)}{g(y)} + \frac{\rho'(y)}{\rho(y)} \right) \Phi_k(y) \right) \right) \]
\[ - \frac{n(n+1)}{2l(y)} - G_2(y) - \frac{h}{2} (1 + (-1)^n) \].

This is a direct formula for calculating \( \mu_n \) in terms of the functions \( \Phi_k \) and \( \Psi_k \). A recurrent formula for \( \mu_n \) can be obtained from (3.13). We have
\[ \mu_{-1}(y) = \frac{G_2(y)}{2\rho(y)}, \]  
\[ \mu_0(y) = \sqrt{\frac{p(y)}{r(y)}} \left( \alpha'_0(y) + \frac{\rho'(y)}{\rho(y)} \alpha_0(y) \right) - \frac{G_1(y)}{2\rho(y)} = \sqrt{\frac{p(y)}{r(y)}} \left( \frac{(g(y)\rho(y))'}{2\rho(y)} \right) - \frac{G_1(y)}{2\rho(y)}, \]  
and
\[ \mu_n(y) = \frac{n\alpha_n(y)}{l(y)} + \sqrt{\frac{p(y)}{r(y)}} \left( \alpha'_n(y) + \frac{\rho'(y)}{\rho(y)} \alpha_n(y) \right) \]
\[ + \frac{2n+1}{2n-3} \left( \mu_{n-2}(y) - \sqrt{\frac{p(y)}{r(y)}} \left( \alpha'_{n-2}(y) + \frac{\rho'(y)}{\rho(y)} \alpha_{n-2}(y) \right) + \frac{n-1}{l(y)} \alpha_{n-2}(y) \right), \quad n = 1, 2, \ldots. \]  

One may also use
\[ \mu_1(y) = \frac{\alpha_1(y)}{l(y)} + \sqrt{\frac{p(y)}{r(y)}} \left( \alpha'_1(y) + \frac{\rho'(y)}{\rho(y)} \alpha_1(y) \right) - \frac{3G_2(y)}{2\rho(y)}. \]  

### 6 Computation formulas for the coefficients

Besides the direct formulas (4.3) and (5.5) for the coefficients \( \alpha_n \) and \( \mu_n \) appearing in the representations (4.1), (4.2), (5.1) and (5.2) it is convenient to have formulas more appropriate for practical computation. The main drawback of formulas (4.3) and (5.5) for numerical computing is the presence of the Legendre polynomial coefficients \( l_{k,n} \) which grow rather fast with a growing \( n \). Here we derive a recurrent integration procedure for computing \( \alpha_n \) and \( \mu_n \), convenient for numerical applications.

Formulas from Remark 3.4 can be used for writing the recurrent integration procedure aimed to compute the functions
\[ \Sigma_n(y) := L^{-1} [\sigma_n(x)] = l^n(y)\alpha_n(y) \quad \text{and} \quad \Upsilon_n(y) := L^{-1} [\tau_n(x)] = l^n(y)\mu_n(y). \]  

From (3.15) we obtain
\[ \Sigma_n(y) = \frac{2n+1}{2n-3} \left( l^2(y)\Sigma_{n-2}(y) + c_n L^{-1} [f(x)\theta_n(x)] \right), \]  
where \( c_n = 1 \) if \( n = 1 \) and \( c_n = 2(2n-1) \) otherwise.
Denote \( \bar{\theta}_n(y) := \theta_n(l(y)) \). Then \( L^{-1} \left[ f(x)\theta_n(x) \right] = g(y)\bar{\theta}_n(y) \). Hence

\[
\Sigma_n(y) = \frac{2n + 1}{2n - 3} \left( l^2(y)\Sigma_{n-2}(y) + c_n g(y)\bar{\theta}_n(y) \right). \tag{6.2}
\]

Analogously, for \( n \in \mathbb{N} \),

\[
\Upsilon_n(y) = \frac{2n + 1}{2n - 3} \left( l^2(y)\Upsilon_{n-2}(y) + c_n \left( \sqrt{\frac{p(\tau)}{r(\tau)}} \left( g'(\tau)\rho(\tau) + g(\tau)\rho'(\tau) \right) \bar{\theta}_n(\tau) + \frac{\bar{\eta}_n(\tau)}{\rho(\tau)} \right) + (c_n - 2n + 1) l(y)\Sigma_{n-2}(y) \right) \tag{6.3}
\]

where \( \bar{\eta}_n(y) := \eta_n(l(y)) \).

A simple change of the integration variable \( t = l(\tau) \) in (6.14) gives us the equalities

\[
\bar{\eta}_n(y) = \int_A^y \left( l(\tau) \left( g'(\tau)\rho(\tau) + g(\tau)\rho'(\tau) \right) + (n - 1)\rho(\tau)g(\tau) \sqrt{\frac{r(\tau)}{p(\tau)}} \right) \rho(\tau)\Sigma_{n-2}(\tau) d\tau \tag{6.4}
\]

and

\[
\bar{\theta}_n(y) = \int_A^y \left( \frac{l(\tau)\Sigma_{n-2}(\tau)}{p(\tau)} - \frac{\bar{\eta}_n(\tau)}{\rho(\tau)} \right) \sqrt{\frac{r(\tau)}{p(\tau)}} d\tau. \tag{6.5}
\]

7 Description of the numerical algorithm

Numerical solution of equation (2.1) for different values of \( \lambda \) can be computed following the sequence:

1. Find a nonvanishing solution \( g \) of (2.6) on \([A, B]\) satisfying the initial condition (2.7). The solution \( g \) can be constructed using the SPPS representation, see, e.g., [14] for details, or by means of any other numerical method.

2. Compute the constant \( h \) from (2.8), \( \alpha_{-1} \) and \( \alpha_0 \) from (4.13), \( G_1 \) and \( G_2 \) from (5.3) and (5.4), \( \mu_{-1} \) and \( \mu_0 \) from (5.6) and (5.7).

3. Compute the set of functions \( \left\{ \Sigma_n, \Upsilon_n, \bar{\eta}_n, \bar{\theta}_n \right\} \) which gives us the coefficients \( \alpha_n = \Sigma_n/l^n \) and \( \mu_n = \Upsilon_n/l^n \).

4. Compute the approximations of the solutions \( v_1 \) and \( v_2 \) and of their derivatives \( v'_1 \) and \( v'_2 \) using (4.1), (4.2) and (5.1), (5.2) with the infinite series replaced by corresponding partial sums.

5. Use the initial conditions (4.1) and (4.5) satisfied by \( v_1 \) and \( v_2 \) to obtain a solution satisfying initial conditions prescribed for solving an initial or boundary value problem and/or a spectral problem related to (2.1).

We refer the reader to [17], [11], [13] for implementation details regarding the recurrent integration and computation of Bessel functions.

Additionally we would like to point out that numerical computation of the coefficients \( \alpha_n \) and \( \mu_n \) either via direct formulas (4.3) and (5.5) or via recurrent formulas (6.1), (6.2) and (6.3) can be tricky for values of \( y \) near the point \( y = A \). One of the reasons is that in recursive formulas an absolute error in any coefficient \( \alpha_n \) propagates to all the following coefficients \( \alpha_{n+2k} \) and in the
direct formulas absolute errors in the first functions $\Phi_k$ are get multiplied by quite large Legendre polynomials' coefficients $l_{k,n}$. Another reason is the division by large powers of $l(y)$ in both (6.1) and (4.3), (5.5). I.e., the coefficients $\alpha_n$ and $\mu_n$ possess absolute errors which we can not expect to decrease as $n \to \infty$, while the absolute values of the coefficients $\alpha_n$ and $\mu_n$ decay as $n \to \infty$ and are bounded by decaying functions as $y \to A$, see Proposition A.3 and Corollary A.4. That is, the computed coefficients will possess large relative errors especially near the point $y = A$.

One possibility to overcome the difficulties mentioned above is to change the values of the computed coefficients $\alpha_n$ and $\mu_n$ near $y = A$ by zero, i.e., we take $\alpha_n(y) = 0$ for all $A \leq y \leq y_n$ and $\mu_n(y) = 0$ for all $A \leq y \leq \tilde{y}_n$. The numbers $y_n$ and $\tilde{y}_n$ may be estimated using the following equalities (which easily follow from (A.2), (A.3), and (A.4) by applying the operator $L^{-1}$ and (1.10)).

$$\sum_{n=0}^{\infty} \frac{\alpha_n(y)}{l(y)} = \frac{G_1(y) + G_2(y)}{2\rho(y)}, \quad \sum_{n=0}^{\infty} \frac{(-1)^n \alpha_n(y)}{l(y)} = \frac{h}{2\rho(y)} \quad (7.1)$$

and

$$\sum_{n=0}^{\infty} \frac{\mu_n(y)}{l(y)} = \frac{q(y)}{4\rho(y)r(y)} - \frac{1}{4r(y)} \left[ p(y) \left( \frac{1}{\rho(y)} \right) \right]' + \frac{hG_2(y) + G_2^2(y)}{2\rho(y)}, \quad (7.2)$$

$$= \frac{1}{4\rho(y)} \left( \frac{q(A)}{r(A)} - \frac{\rho(A)}{r(A)} \left[ p(y) \left( \frac{1}{\rho(y)} \right) \right]' \right)_{y=A} + \frac{hG_2(y)}{2\rho(y)} \quad (7.3)$$

One computes differences between the right-hand sides of (7.1), (7.2), (7.3) and partial sums of the series from the left-hand sides, and finds the moment when these differences cease to decrease and reach some floor value as $N$ (the number of terms in the partial sums) grows. Analyzing these values of $N$ for each $y$ one may estimate the values $y_n$ and $\tilde{y}_n$.

Another simple rule for choosing $y_n$ and $\tilde{y}_n$ which we found being quite acceptable numerically consists in the following. After computing a coefficient $\alpha_n$ for some $n$, we take $y_n$ as a point in a neighborhood of $y = A$ where $\alpha_n(y) \neq 0$ and $|\alpha_n(y)|$ attains its minimum. The same procedure for the coefficients $\mu_n$. As an explanation for this rule we refer to Proposition A.3 and Corollary A.4 from which it follows that the coefficients $\alpha_n$ and $\mu_n$ are bounded by some powers of $l(y)$ near $y = A$ and $l(y) \to 0$ as $y \to A$.

It is worth mentioning that as follows from the inequality \[|j_n(z)| \leq \sqrt{\pi} \frac{|z|^n}{2^{n+1}} \frac{e^{-\frac{1}{2} |z|^2}}{\Gamma(n + 3/2)}, \quad z \in \mathbb{C},\]

the values of the function $j_n(z)$ for small $z$ and large $n$ are so small (for example, $j_{40}(1) \approx 1.5 \cdot 10^{-61}$, $j_{40}(10) \approx 8.4 \cdot 10^{-22}$) that even huge errors in the coefficients $\alpha_n(y)$ and $\mu_n(y)$ in a neighborhood of $y = A$ do not lead to significant errors in the approximate solutions. Only for large values of $\omega$ (corresponding to 100th eigenvalue and further) the error can be noticeable, see Section 8 for an illustration.

8 Numerical experiments

We implemented the algorithm from Section 7 in Matlab 2012 in machine precision arithmetics. All the calculations were performed as was described in [11], [13], [15]. We opted for a straightforward implementation to illustrate that the proposed method is capable to produce highly accurate results.
as is. Clearly it can benefit even more being combined with such techniques as interval subdivision etc.

We considered the following equation \[11\],\[8\], Eqn. 2.273(11)]
\[
\begin{align*}
    u'' - 2u' + u &= -\lambda(y^2 + 1)u, \\
    y &\in [0, 2]
\end{align*}
\] (8.1)
together with the boundary conditions
\[
    u(0) - u'(0) = 0, \quad u(2) + u'(2) = 0.
\] (8.2)

Equation (8.1) can be transformed into the form (2.1) with
\[
    p(y) = e^{-2y}, \quad q(y) = -e^{-2y} \quad \text{and} \quad r(y) = (y^2 + 1)e^{-2y}.
\]

The algorithm from our previous paper \[11\] was able to compute the first 100 eigenvalues for this problem with the maximum absolute error of \(4.7 \cdot 10^{-7}\) and maximum relative error of \(8.5 \cdot 10^{-9}\). Though such accuracy is quite impressive, it is far from the limitations of the machine double precision, when one can expect relative errors as low as \(2.3 \cdot 10^{-16}\). This was a motivation for us to illustrate the numerical performance of the new solution representations by showing that they can produce significantly more accurate results for the same problem requiring similar computation resources.

We used 2001 uniformly spaced points to represent all the functions involved and computed the coefficients \(\alpha_n\) and \(\mu_n\) for \(n \leq 50\). The coefficients were computed “as is”, without any special care about their behavior near \(y = A\). Criteria based on the equalities (7.1)–(7.3) showed that optimal value for \(N\) for the approximate solutions was \(N = 38\), which was used to compute the first 100 eigenvalues. On Figure 1 we present absolute and relative errors of the computed eigenvalues. The maximal absolute error was \(1.3 \cdot 10^{-11}\), and the maximal relative error was \(2.5 \cdot 10^{-15}\). The computation time on a computer equipped with Intel i7-3770 CPU was about 0.25 seconds (a significant speed-up was achieved by computing the spherical Bessel functions recurrently, see \[3\], \[7\] and \[13\] for details).

![Figure 1: Absolute and relative errors of the first 100 eigenvalues for the spectral problem (8.1), (8.2).](image)

On Figure 2 we illustrate the difficulty in the computation of the coefficients \(\alpha_n\) and \(\mu_n\) explained at the end of Section 7. Direct implementation of the recurrent formulas (6.1), (6.2) leads to large errors in the coefficients in a neighborhood of \(y = 0\), while the coefficients computed using the proposed workaround remain bounded in the same region.
Figure 2: Absolute values of the coefficients $\alpha_k(y)$ for $k = 4, 10, 15, 20$. On the left plot: calculated directly using the recurrent formulas (6.1), (6.2). Note the growth of the values $|\alpha_k(y)|$ as $y \to 0$, especially for large values of $k$. On the right plot: calculated using the workaround proposed at the end of Section 7.

In the last experiment we verified the accuracy of the approximate solutions. One of the exact solutions of equation (8.1) has the form

$$u(y) = \exp \left( y - \frac{i y^2 \omega}{2} \right) \, _1 F_1 \left( 1 + \frac{i \omega}{4}, \frac{1}{2}, i y^2 \omega \right),$$

where $\lambda = \omega^2$ and $\, _1 F_1$ is the Kummer confluent hypergeometric function. It satisfies the initial conditions $u(0) = u'(0) = 1$. We calculated this solution numerically for three different values of $\omega$, 52, 105 and 210 (being close to 50th, 100th and 200th eigenvalues respectively). $N = 38$ was used for the approximate solutions. The coefficients $\alpha_n$ and $\mu_n$ were computed in two different ways: directly using the recurrent formulas and with a special care for small values of $y$ (as was explained in Section 7). On Figure 3 we present the absolute errors of the approximate solutions. We omitted the case $\omega = 52$ since the errors are indistinguishable on the plots. For $\omega = 105$ or $\omega = 210$ one starts to observe additional errors for small values of $y$ due to errors in the coefficients $\alpha_n$ and $\mu_n$.

A Error and decay rate estimates

In this appendix some estimates for the functions $\varepsilon_N$ and $\varepsilon_{1,N}$ from Theorems 3.1 and 3.2 are presented. Also decay rate estimates and bounds near $x = 0$ for the coefficients $\beta_n$ and $\gamma_n$ are obtained in dependence on the smoothness of the potential $Q$. The estimates are from [13] with some additional improvements obtained using ideas from [15].

It is well known (see, e.g., [19], [20], [21], [23]) that the solutions $c(\omega, x)$ and $s(\omega, x)$ of (2.3) satisfying the initial conditions (3.1) can be represented as

$$c(\omega, x) = \cos \omega x + \int_{-x}^{x} K(x, t) \cos \omega t \, dt$$

and

$$s(\omega, x) = \sin \omega x + \int_{-x}^{x} K(x, t) \sin \omega t \, dt,$$
Absolute errors of the approximate solution for $\omega = 105$.

Figure 3: Absolute errors of the approximate solution $u_N(\omega, y)$. On the left: using the coefficients $\alpha_n(y)$ calculated directly, without any special treatment for small values of $y$. On the right: using the coefficients $\alpha_n(y)$ calculated applying the workaround proposed at the end of Section 7.

i.e., as images of the functions $\cos \omega t$ and $\sin \omega t$ under the action of the so-called transmutation operator $T$. This operator is defined on an arbitrary integrable function by the rule

$$ Tu(x) = u(x) + \int_{-x}^{x} K(x, t) u(t) \, dt. \quad (A.1) $$

Its integral kernel $K$ satisfies the equalities

$$ K(x, x) = \frac{h}{2} + \frac{1}{2} \int_{0}^{x} Q(s) \, ds, \quad K(x, -x) = \frac{h}{2}, \quad (A.2) $$

and the derivative $\partial_x K = K_1$ satisfies the equalities (see [18])

$$ K_1(x, x) = \frac{Q(x)}{4} + \frac{h}{4} \int_{0}^{x} Q(s) \, ds + \frac{1}{8} \left( \int_{0}^{x} Q(s) \, ds \right)^2, \quad K_1(x, -x) = \frac{1}{4} \left( Q(0) + h \int_{0}^{x} Q(s) \, ds \right). \quad (A.3) $$

The integral kernel $K$ is one degree smoother than the potential $Q$. To be more precise, let $Q \in W^{p+1}_{\infty}[0, b]$, $p \geq 0$, i.e., the function $Q$ possesses $p$ derivatives, the last one belonging to $L_{\infty}(0, b)$. In such case the integral kernel $K$ possesses $p+1$ derivative with respect to each variable. In particular, for each $x > 0$, $K(x, \cdot) \in W^{p+1}_{\infty}[-x, x]$ and the norms $\|\partial_t^{p+1} K(x, t)\|_{L_{\infty}(-x,x)}$ are bounded on $[0, b]$.  

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The following result shows that the coefficients $\beta_n$ and $\gamma_n$ defined by (3.4) and (3.11) are the Fourier-Legendre coefficients of the integral kernel $K$ and its derivative $K_1 := \partial_t K$, respectively.

**Theorem A.1** [(13)]. Let $Q \in L_\infty(0,b)$. The transmutation kernel $K$ and its derivative $K_1$ have the form

$$K(x,t) = \sum_{j=0}^\infty \frac{\beta_j(x)}{x} P_j\left(\frac{t}{x}\right) \quad \text{and} \quad K_1(x,t) = \sum_{j=0}^\infty \frac{\gamma_j(x)}{x} P_j\left(\frac{t}{x}\right),$$  

(A.4)

here $P_n$ denotes the classical Legendre polynomials. The coefficients $\beta_n$ and $\gamma_n$, $n \geq 0$, can be recovered using the formulas

$$\beta_n(x) = \frac{2n+1}{2} \int_{-x}^x K(x,t)P_n\left(\frac{t}{x}\right) \, dt \quad \text{and} \quad \gamma_n(x) = \frac{2n+1}{2} \int_{-x}^x K_1(x,t)P_n\left(\frac{t}{x}\right) \, dt.$$  

(A.5)

Denote by $K_N$ and $K_{1,N}$ partial sums of the series (A.4). Let $Q \in W^p\_\infty[0,b]$, $p \geq 0$. Define

$$M := \sup_{0 < x \leq b} \|\partial_t^{p+1}K(x,\cdot)\|_{L_\infty(-x,x)} \quad \text{and} \quad M_1 := \sup_{0 < x \leq b} \|\partial_t^{p}K_1(x,\cdot)\|_{L_\infty(-x,x)}.$$  

(A.6)

As was mentioned earlier, both suprema exist and are finite numbers. The following convergence rate estimates hold.

**Proposition A.2.** Let $Q \in W^p\_\infty[0,b]$, $p \geq 0$. Then there exist constants $c_p$ and $d_p$ independent of $Q$ and $N$, such that for all $x > 0$ the following inequalities hold

$$\|K(x,\cdot) - K_N(x,\cdot)\|_{L_2(-x,x)} \leq \frac{c_p M x^{p+3/2}}{N^{p+1}}, \quad N \geq p + 2,$$  

(A.7)

and

$$\|K_1(x,\cdot) - K_{1,N}(x,\cdot)\|_{L_2(-x,x)} \leq \frac{d_p M_1 x^{p+1/2}}{N^{p}}, \quad N \geq p + 1.$$  

(A.8)

**Proof.** Let $x > 0$ be fixed. Consider functions $g(z) := K(x,xz)$ and $g_N(z) := K_N(x,xz)$ defined on $[-1,1]$. The function $g_N$ is a partial sum of the Fourier-Legendre series for the function $g$, hence $g_N$ coincides with the $N$-th order polynomial best $L_2$ approximation of the function $g$. Since the integral kernel $K$ possesses $p + 1$ derivatives with respect to the second variable with the last derivative belonging to $L_\infty(-x,x)$, we have that $g \in W^{p+1}_\infty[-1,1] \subset W^{p+1}_2[-1,1]$. Theorem 6.2 from [5] states that there exists a universal constant $\tilde{c}_p$ such that for every $N > p + 1$

$$\|g - g_N\|_{L_2(-1,1)} \leq \frac{\tilde{c}_p}{N^{p+1}} \omega\left(g^{(p+1)}; \frac{1}{N}\right)^{1/2} \leq \frac{2\tilde{c}_p}{N^{p+1}} \|g^{(p+1)}\|_{L_2(-1,1)},$$

where $\omega$ is the modulus of continuity.

By the definition $g^{(p+1)}(z) = x^{p+1} \partial_t^{p+1}K(x,t)|_{t=xz} = x^{p+1}K^{(p+1)}_2(x,xz)$, hence

$$\|K(x,\cdot) - K_N(x,\cdot)\|_{L_2(-x,x)} = \sqrt{x} \|g - g_N\|_{L_2(-1,1)} \leq \frac{2\tilde{c}_p \sqrt{x}}{N^{p+1}} \|g^{(p+1)}\|_{L_2(-1,1)}$$

$$= \frac{2\tilde{c}_p x^{p+3/2}}{N^{p+1}} \|K^{(p+1)}_2(x,x\cdot)\|_{L_2(-1,1)} \leq \frac{2\tilde{c}_p}{N^{p+1}} \frac{M x^{p+3/2}}{N^{p+1}},$$

where we used that $\|K^{(p+1)}_2(x,x\cdot)\|_{L_2(-1,1)} \leq \sqrt{2}M$ due to (A.6).

The second estimate (A.8) can be obtained similarly.
Estimates \( A.7 \) and \( A.8 \) provide upper bounds for the error functions \( \varepsilon_N \) and \( \varepsilon_{1,N} \) from Theorems 3.1 and 3.2. Indeed, the approximate solutions \( c_N \) and \( s_N \) are obtained by changing \( K \) by \( K_N \) in \( (A.1) \). Hence by the Cauchy-Schwarz inequality we have

\[
|c(\omega, x) - c_N(\omega, x)| \leq \left| \int_{-x}^{x} (K(x, t) - K_N(x, t)) \cos \omega t \, dt \right|
\]

\[
\leq \| K(x, \cdot) - K_N(x, \cdot) \|_{L_2(-x, x)} \cdot \left( \int_{-x}^{x} |\cos \omega t|^2 \, dt \right)^{1/2} \leq \frac{\sqrt{2}c_p M x^{p+2}}{N^{p+1}} \tag{A.9}
\]

for any \( \omega \in \mathbb{R} \). The estimates for the function \( \varepsilon_{1,N} \) follows similarly by using corresponding estimates for the derivative \( K_1 \).

The following proposition provides estimates of the decay rate of the coefficients \( \beta_k \) and \( \gamma_k \) and their behavior near \( x = 0 \).

**Proposition A.3.** Let \( Q \in W^p_x[0, b], p \geq 0 \). There exist constants \( C_p \) and \( D_p \) (independent of \( N \)) such that

\[
|\beta_N(x)| \leq \frac{C_p x^{p+2}}{(N - 1)^{p+1/2}}, \quad N \geq p + 1 \tag{A.10}
\]

and

\[
|\gamma_N(x)| \leq \frac{D_p x^{p+1}}{(N - 1)^{p-1/2}}, \quad N \geq p \tag{A.11}
\]

**Proof.** We obtain using \( (A.5) \) and \( (A.7) \), the fact that the Legendre polynomial \( P_n \) is orthogonal to any polynomial of degree less than \( N \) and the Cauchy-Schwarz inequality that

\[
|\beta_N(x)| = \frac{2N + 1}{2} \left| \int_{-x}^{x} K(x, t) P_N \left( \frac{t}{x} \right) \, dt \right| \leq \frac{2N + 1}{2} \int_{-x}^{x} \left| (K(x, t) - K_{N-1}(x, t)) P_N \left( \frac{t}{x} \right) \right| \, dt
\]

\[
\leq \frac{2N + 1}{2} \| K(x, \cdot) - K_{N-1}(x, \cdot) \|_{L_2(-x, x)} \cdot \sqrt{\frac{2x}{2N + 1}} \leq \sqrt{\frac{2N + 1}{2} \frac{c_p M x^{p+2}}{(N - 1)^{p+1}}}
\]

The proof of the second estimate \( (A.11) \) is similar. \( \square \)

The following bound for the behavior of the first coefficients near \( x = 0 \) is valid.

**Corollary A.4.** Let \( Q \in W^p_x[0, b], p \geq 0 \). Then

\[
|\beta_n(x)| \leq c_n x^{n+1}, \quad n \leq p + 1 \tag{A.12}
\]

\[
|\gamma_n(x)| \leq d_n x^{n+1}, \quad n \leq p \tag{A.13}
\]

where \( c_n \) and \( d_n \) are some constants dependent on \( Q \).

Sufficient conditions for the smoothness of the transformed potential \( Q \) in terms of the coefficients \( p, q \) and \( r \) can be easily obtained from \( (2.4) \).

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