Construction of a transmutation for the one-dimensional Schrödinger operator and a representation for solutions

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Abstract
A new representation for solutions of the one-dimensional Schrödinger equation
\[-u'' + q(x)u = \omega^2 u\]
is obtained in the form of a series possessing the following attractive feature. The truncation error is \(\omega\)-independent for all \(\omega \in \mathbb{R}\). For the coefficients of the series simple recurrent integration formulas are obtained which make the new representation applicable for computation.

1 Introduction
In the present work a new representation for solutions of the one-dimensional Schrödinger equation
\[-u'' + q(x)u = \omega^2 u\] (1)
is obtained in the form of a series possessing the following attractive feature. If \(u_N(\omega, x)\) denotes the truncated series and \(u(\omega, x)\) the exact solution, the following inequality is valid for any \(\omega \in \mathbb{R}\), \(|u(\omega, x) - u_N(\omega, x)| \leq \varepsilon_N(x)\), where \(\varepsilon_N\) is a nonnegative function independent of \(\omega\) and \(\varepsilon_N(x) \to 0\) when \(N \to \infty\). For the coefficients of the series simple recurrent integration formulas are obtained which make the new representation applicable for computation.

In the recent work [6] a representation for solutions of (1) possessing the described above feature was proposed in a completely different form. Both representations are united by the fact that they are obtained with the use of a transmutation (transformation) operator. In [6] the solution \(u\) of (1) satisfying the initial conditions
\[u(0) = 1, \quad u'(0) = -i\omega\]
was considered in the form
\[u(\omega, x) = e^{-i\omega x} + \int_{-x}^{x} K(x, y)e^{-i\omega y} dy,\]

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well known from [11], [12] and numerous other publications. The kernel \( K \) was found in [6] in the form of a Fourier-Legendre series which led to a representation of \( u(\omega, x) \) in the form of a Neumann series of Bessel functions (NSBF). In the present work we explore another possibility of representing \( u(\omega, x) \) as a result of action of a transmutation operator. Namely, an elementary reasoning (see the next section) based on the well known facts from the scattering theory leads to another representation of \( u(\omega, x) \) in the form

\[
u(\omega, x) = e^{-i\omega x} + \int_{-\infty}^{x} A(x, y)e^{-i\omega y}dy \]

where the kernel \( A(x, \cdot) \in L_2(-\infty, x) \) is that arising in the scattering theory associated with [1], see, e.g., [1]. Since the integral in (2) is taken over a semi-infinite interval it is natural to look for \( A(x, \cdot) \) in the form of a Fourier-Laguerre series. This is done in the present work, and as a corollary a new representation for solutions of (1) is obtained. For \( \omega \)-independent coefficients of the representation a direct formula is derived in terms of so-called formal powers arising in spectral parameter power series (SPPS) method [3], [7], [8]. Moreover, a much more convenient for computing recurrent integration formula is obtained as well, which in practice allows one to compute thousands of the coefficients. We illustrate several features of the new representation numerically on a simple test problem. All the computations reported here took not more than several seconds performed in Matlab 2012, including those which involved computation of up to \( 10^5 \) coefficients. Although this paper is not about a new numerical algorithm, and we do not discuss details of its implementation, our numerical results show that the new representation can be of interest for practical computation.

Finally, the new representation can be extended onto a general Sturm-Liouville equation as well as onto the perturbed Bessel equation (see [9] and [10] where it was done for the NSBF representation).

Besides this Introduction the paper contains four sections. In Section 2 we obtain the Fourier-Laguerre expansion of the kernel \( A \). In Section 3 we prove the main result of this work, the new representation for solutions of (1). In Section 4 we derive a recurrent integration procedure for computing the coefficients in the representation. Section 5 contains some numerical illustrations.

## 2 Construction of a transmutation

Consider the equation

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

on a finite interval \((0, d)\). We suppose that \( q \) is a real valued, measurable function. The solution of (3) satisfying the initial conditions

\[u(0) = 1, \quad u'(0) = -i\omega, \]

will be denoted as \( u(\omega, x) \). We consider \( \omega \in \mathbb{R} \).

One can extend \( q \) by zero onto the whole line, and \( u(\omega, x) \) by \( e^{-i\omega x} \) onto the half-line \((-\infty, 0)\). Then \( u(\omega, x) \) can be regarded as a Jost solution of (3) satisfying the asymptotic
relation (which is in fact an equality in our case) \( u(\omega, x) \sim e^{-i\omega x} \) when \( x \to -\infty \). Hence, it is known (see, e.g., [1]) that there exists such a function \( A(x, \cdot) \in L_2(-\infty, x) \) that
\[
\begin{align*}
  u(\omega, x) &= e^{-i\omega x} + \int_{-\infty}^{x} A(x, y)e^{-i\omega y}dy \\
  &\quad \text{for all} \ \omega.
\end{align*}
\]

This integral representation of \( u(\omega, x) \) can be viewed as action of an operator of transmutation (transformation) with the kernel \( A(x, y) \) on the solution \( e^{-i\omega x} \) of the elementary equation \(-u'' = \omega^2 u\). Denote this operator by \( A[v](x) := v(x) + \int_{-\infty}^{x} A(x, y)v(y)dy \).

Note that (see, e.g., [1])
\[
A(x, x) = \frac{1}{2} \int_{0}^{x} q(y)dy.
\]

By a change of the integration variable equality (5) can be written as follows
\[
\begin{align*}
u(\omega, x) &= e^{-i\omega x} \left( 1 + \int_{0}^{\infty} A(x, x-t)e^{i\omega t}dt \right).
\end{align*}
\]

Let us represent the kernel \( A(x, x-t) \) in the form \( A(x, x-t) = a(x, t)e^{-t} \). The function \( a(x, \cdot) \) then belongs to the space \( L_2(0, \infty; e^{-t}) \) equipped with the scalar product \( \langle u, v \rangle := \int_{0}^{\infty} u(t)v(t)e^{-t}dt \) and the norm \( \|u\| := \sqrt{\langle u, u \rangle} \). Thus, for any \( x \in [0, d] \) the function \( a(x, \cdot) \) admits a Fourier-Laguerre expansion convergent in this norm,
\[
a(x, t) = \sum_{n=0}^{\infty} a_n(x)L_n(t),
\]
where \( L_n \) stands for the Laguerre polynomial of order \( n \), and hence
\[
A(x, y) = \sum_{n=0}^{\infty} a_n(x)L_n(x-y)e^{-(x-y)}.
\]

We note that due to (6) and the fact that \( L_n(0) = 1 \) we have the equality
\[
\sum_{n=0}^{\infty} a_n(x) = \frac{1}{2} \int_{0}^{x} q(y)dy.
\]

In order to find formulas for the coefficients \( a_n \) we introduce first the following notations.

Throughout the paper we suppose that \( f_0 \) is a solution of the equation
\[
\begin{align*}
f'' - q(x)f &= 0
\end{align*}
\]
satisfying the initial conditions
\[
\begin{align*}
f_0(0) &= 1, \\ f_0'(0) &= 0.
\end{align*}
\]

Consider two sequences of recursive integrals (see [4], [7])
\[
\begin{align*}
X^{(0)}(x) &\equiv 1, \\
X^{(n)}(x) &= n \int_{0}^{x} X^{(n-1)}(s) \left(f_0^2(s)\right)^{(-1)^n} ds, \quad n = 1, 2, \ldots
\end{align*}
\]
and
\[
\begin{align*}
\tilde{X}^{(0)} &\equiv 1, \\
\tilde{X}^{(n)}(x) &= n \int_{0}^{x} \tilde{X}^{(n-1)}(s) \left(f_0^2(s)\right)^{(-1)^{n-1}} ds, \quad n = 1, 2, \ldots
\end{align*}
\]
Definition 1. The family of functions $\{\varphi_k\}_{k=0}^{\infty}$ constructed according to the rule

$$\varphi_k(x) = \begin{cases} f_0(x)X^{(k)}(x), & k \text{ odd}, \\ f_0(x)\tilde{X}^{(k)}(x), & k \text{ even} \end{cases}$$

(12)

is called the system of formal powers associated with $f_0$.

Remark 2. If $f_0$ has zeros some of the recurrent integrals (10) or (11) may not exist, although even in that case the formal powers (12) are well defined. It is convenient to construct them in the following way. Take a nonvanishing solution $f$ of (3) such that $f(0) = 1$. For example, $f = f_0 + if_1$ where $f_1$ is a solution of (3) satisfying $f_1(0) = 0$, $f_1'(0) = 1$. Since $q$ is real valued such $f$ does not vanish. Then (see [8, Proposition 4.7])

$$\varphi_k = \begin{cases} \Phi_k, & k \text{ odd}, \\ \Phi_k - \frac{f(0)}{k+1} \Phi_{k+1}, & k \text{ even}, \end{cases}$$

where $\Phi_k$ are formal powers associated with $f$.

Remark 3. The formal powers arise in the spectral parameter power series (SPPS) representation for solutions of (3) (see [3], [4], [5], [7]). In particular, the solution $u(\omega, x)$ has the form

$$u(\omega, x) = \sum_{n=0}^{\infty} \frac{(-i\omega)^n \varphi_n(x)}{n!}.$$  

(13)

The series converges uniformly both with respect to $x$ on $[0, d]$ and with respect to $\omega$ on any compact subset of the complex plane.

Proposition 4

$$A[x^k] = \varphi_k.$$  

(14)

Proof. From (3) and (13) the following equality follows

$$\sum_{n=0}^{\infty} \frac{(-i\omega)^n \varphi_n(x)}{n!} = \sum_{n=0}^{\infty} \frac{(-i\omega)^n x^n}{n!} + \sum_{n=0}^{\infty} \frac{(-i\omega)^n}{n!} \int_{-\infty}^{x} A(x, y)y^n dy$$

for all $\omega$

from which (14) is obtained by equating expressions at corresponding powers of $\omega$. ■

Proposition 5. The coefficients $a_n$ in (7) have the form

$$a_n(x) = \sum_{j=0}^{n} (-1)^j (\varphi_j(x) - x^j) \sum_{k=j}^{n} (-1)^k \frac{n!}{(n-k)!k!(k-j)!j!} x^{k-j}.$$  

(15)
Proof. Denote by $l_{k,n} := (-1)^k (\frac{n}{k})$ the coefficient at $x^k$ of the Laguerre polynomial $L_n(x)$. Consider the integral

$$
\int_{-\infty}^{x} A(x, y) L_n(x - y) dy = \sum_{n=0}^{\infty} a_m(x) \int_{-\infty}^{x} L_m(x - y) L_n(x - y) e^{-(x-y)} dy
$$

$$
= \sum_{n=0}^{\infty} a_m(x) \int_{0}^{\infty} L_m(t) L_n(t) e^{-t} dt = a_n(x).
$$

Hence

$$
a_n(x) = \int_{-\infty}^{x} A(x, y) L_n(x - y) dy = \sum_{k=0}^{n} l_{k,n} \int_{-\infty}^{x} A(x, y) (x - y)^k dy
$$

$$
= \sum_{k=0}^{n} l_{k,n} \sum_{j=0}^{k} (-1)^j \binom{k}{j} x^{k-j} \int_{-\infty}^{x} A(x, y) y^j dy.
$$

From (14) we have that $\int_{-\infty}^{x} A(x, y) y^j dy = \varphi_j(x) - x^j$, and hence

$$
a_n(x) = \sum_{k=0}^{n} l_{k,n} \sum_{j=0}^{k} (-1)^j \binom{k}{j} x^{k-j} (\varphi_j(x) - x^j)
$$

from where (15) is obtained by changing the order of summation. □

Remark 6 Although formula (15) offers an explicit expression for the coefficients, it is not the best alternative for practical computation. Another representation for $a_n$ suited better for computational purposes is derived in Section 4.

3 A representation for solutions of (3)

Theorem 7 The solution $u(\omega, x)$ of (3) satisfying the initial conditions (4) has the form

$$
u(\omega, x) = e^{-i\omega x} \left( 1 + \sum_{n=0}^{\infty} (-1)^n a_n(x) \frac{(i\omega)^n}{(1 - i\omega)^{n+1}} \right).
$$

(16)

The following estimate is valid for any $\omega \in \mathbb{R}$,

$$
|u(\omega, x) - u_N(\omega, x)| \leq \varepsilon_N(x),
$$

(17)

where

$$
u_N(\omega, x) := e^{-i\omega x} \left( 1 + \sum_{n=0}^{N} (-1)^n a_n(x) \frac{(i\omega)^n}{(1 - i\omega)^{n+1}} \right),
$$

and $\varepsilon_N(x)$ is a nonnegative function independent of $\omega$ and such that $\varepsilon_N(x) \to 0$ for all $x \in [0, d]$ when $N \to \infty$. 

5
Proof. Consider (5). Substitution of (7) into it gives us the equality

\[ u(\omega, x) = e^{-i\omega x} + \sum_{n=0}^{\infty} a_n(x) \int_{-\infty}^{x} L_n(x-y)e^{-(x-y)}e^{-i\omega y} dy = e^{-i\omega x} \left( 1 + \sum_{n=0}^{\infty} a_n(x) \int_{0}^{\infty} L_n(t)e^{-(1-i\omega)t} dt \right). \]

For the last integral the following equality holds [2, 7.414 (2)]

\[ \int_{0}^{\infty} L_n(t)e^{-(1-i\omega)t} dt = \frac{(-1)^n (i\omega)^n}{(1-i\omega)^{n+1}}, \]

from where we obtain (16).

To prove (17) consider the difference

\[ |u(\omega, x) - u_N(\omega, x)| = \left| \int_{0}^{\infty} e^{-t} (a(x,t) - a_N(x,t)) e^{-i\omega(x-t)} dt \right| \]

\[ = \left| \langle a(x,t) - a_N(x,t), e^{-i\omega(x-t)} \rangle \right|, \]

where \( a_N(x,t) := \sum_{n=0}^{N} a_n(x) L_n(t) \). Application of the Cauchy–Bunyakovsky–Schwarz inequality leads to the inequality

\[ |u(\omega, x) - u_N(\omega, x)| \leq \|a(x,t) - a_N(x,t)\| \|e^{-i\omega(x-t)}\| \]

where obviously \( \|e^{-i\omega(x-t)}\| = 1 \) for \( \omega \in \mathbb{R} \). Now denoting

\[ \varepsilon_N(x) := \|a(x,t) - a_N(x,t)\| = \left( \int_{0}^{\infty} e^{-t} |a(x,t) - a_N(x,t)|^2 dt \right)^{1/2} \]

we obtain (17).

Remark 8 The series (16) can be considered also in the case \( \omega \in \mathbb{C} \), though not for all values of \( \omega \) such attractive estimates as (17) are possible. Indeed, first we note that the function \( e^{i\omega t} \in L_2(0, \infty; e^{-t}) \) if only \( \text{Im} \omega > -1/2 \) and in this case \( \|e^{i\omega t}\| = 1/\sqrt{1 + 2 \text{Im} \omega} \).

Thus, applying the reasoning from the proof of Theorem 7 we obtain

\[ |u(\omega, x) - u_N(\omega, x)| \leq \frac{\varepsilon_N(x) e^{\text{Im} \omega x}}{\sqrt{1 + 2 \text{Im} \omega}}, \]

when \( \text{Im} \omega > -1/2 \).

This estimate is independent of \( \text{Re} \omega \) and is especially attractive when \(-1/2 < \text{Im} \omega \leq 0\). We discuss its applications in Section 5.

4 A recurrent procedure for computing the coefficients \( a_n \)

In order to obtain another way to compute \( a_n \) we substitute (16) into equation (3). Let us stress that it is done formally without discussing the possibility of differentiation of the
series \(16\) with respect to \(x\), and only with the aim to obtain the recurrent formulas which then can be easily checked directly from \(15\).

Differentiating twice \(16\) we obtain the equality

\[
u''(\omega, x) + \omega^2 u(\omega, x) = e^{-i\omega x} \left( \sum_{n=0}^{\infty} a_n''(x) \frac{(-i\omega)^n}{(1 - i\omega)^{n+1}} - 2i\omega \sum_{n=0}^{\infty} a_n'(x) \frac{(-i\omega)^n}{(1 - i\omega)^{n+1}} \right).
\]

Using \(3\) on the left-hand side we have that

\[
q(x) \left( 1 + \sum_{n=0}^{\infty} a_n(x) \frac{(-i\omega)^n}{(1 - i\omega)^{n+1}} \right) = \sum_{n=0}^{\infty} \left( a_n''(x) \frac{(-i\omega)^n}{(1 - i\omega)^{n+1}} + 2a_n'(x) \frac{(-i\omega)^n}{(1 - i\omega)^{n+1}} \right).
\]

Denote \(z := \frac{i\omega}{1 - i\omega}\). Then the last equality can be written as follows

\[
q(x) \left( 1 + \frac{1 + z}{z} \sum_{n=0}^{\infty} (-1)^n a_n(x) z^{n+1} \right) = \sum_{n=0}^{\infty} \left( (-1)^n a_n''(x) \frac{1 + z}{z} z^{n+1} + (-1)^{n+1} 2a_n'(x) z^{n+1} \right)
\]

or

\[
q(x) \left( 1 + (1 + z) \sum_{n=0}^{\infty} (-1)^n a_n(x) z^n \right) = \sum_{n=0}^{\infty} \left( (-1)^n a_n''(x) (1 + z) z^n + (-1)^{n+1} 2a_n'(x) z^{n+1} \right).
\]

Equating terms corresponding to equal powers of \(z\) we obtain the equalities

\[
L a_n = L a_{n-1} - 2a_{n-1}'
\]

(18)

where \(L := \frac{d^2}{dx^2} - q\). Moreover, from \(15\) it follows that

\[
a_0 = f_0 - 1,
\]

(19)

and

\[
a_n(0) = a_n'(0) = 0
\]

(20)

for all \(n = 0, 1, \ldots\). From here a simple recurrent procedure for computing the coefficients \(a_n\) can be proposed which is formulated as the following statement.

**Proposition 9** The coefficients \(a_n\) in \(7\) and \(10\) can be calculated by means of the following recurrent integration procedure

\[
a_n(x) = a_{n-1}(x) - 2f(x) \int_0^x a_{n-1}(s) ds + 2 f(x) \int_0^x \frac{1}{f^2(t)} \int_0^t f'(s) a_{n-1}(s) ds
\]

(21)

with \(f\) being any solution of \(3\), nonvanishing on \([0, d]\), see Remark 2, and \(a_0\) defined by \(19\).

**Proof.** One of the possibilities to write down a solution of the inhomogeneous equation \(L a_n = g\) satisfying \(20\) is using the formula

\[
a_n(x) = f(x) \int_0^x \frac{1}{f^2(t)} \int_0^t f(s) g(s) ds.
\]

Its application to \(18\) gives us the following equality

\[
a_n(x) = a_{n-1}(x) - 2f(x) \int_0^x \frac{1}{f^2(t)} \int_0^t f(s) a_{n-1}'(s) ds
\]

which after an integration by parts can be written in the form \(21\). \(\blacksquare\)
5 Numerical illustrations

Example 10 Consider $q \equiv 1$. This elementary example is sufficient to show main features of the proposed representation for solutions of (3). Note that although the solutions can be written in a closed form the coefficients $a_n$ are rather nontrivial since $f_0(x) = \cosh x$ and the recurrent integrals in (12) or in (21) can be calculated explicitly only for few first coefficients. Thus, formula (21) was implemented numerically, and first we notice that it allows one to compute, if necessary, dozens of thousands of the coefficients $a_n$. We illustrate this observation by Fig. 1 and Fig. 2 on which the difference $\max_{x \in [0,1]} \left| \frac{1}{2} \int_0^x q(y) \, dy - \sum_{n=0}^N a_n(x) \right|$ is presented for $N$ from zero to ten thousands and from ten thousands one to one hundred thousands respectively. Both graphs show that the sum $\sum_{n=0}^N a_n(x)$ with the computed coefficients $a_n$ tends to $\frac{1}{2} \int_0^x q(y) \, dy$ according to (8) still for large $N$. We observe a quite slow decay of the coefficients $a_n$. On Fig. 3 the magnitude $\max_{x \in [0,1]} |a_n(x)|$ is presented for $n = 0, 1, \ldots, 100$ while on Fig. 4 the same magnitude is presented for $n = 101, \ldots, 1000$.

Fig. 5 shows the absolute error of the approximate solution for $N = 100$ while Fig. 6 shows the same magnitude but for $N = 10^4$. Finally, we illustrate the uniformity of the approximation with respect to $\omega \in \mathbb{R}$ prescribed by (17). On Fig. 7 we show the absolute error of the approximate solution for $N = 100$ on the interval $\omega \in [-1000, 1000]$. It can be observed that the maximum of the error is achieved relatively near the origin, in this case when $|\omega| \approx 10$, and the error decays for large values of $\omega$, for $\omega = \pm 1000$ it is of order $10^{-6}$.

Fig. 8 shows the absolute error of the approximate solution for $N = 10^4$ on the same interval $\omega \in [-1000, 1000]$. Now the maximum of the absolute error though two orders better than in the previous test is achieved when $|\omega| \approx 78$. In the next experiment we chose $\omega = -i/4$, see Remark 8. Already with $N = 30$ the value of both the absolute and the relative errors of the solution was of order $10^{-16}$. That confirms the estimate from Remark 8 and shows that the series (17) converges especially fast when $-1/2 < \text{Im} \omega < 0$ and $\text{Re} \omega = 0$. This can be used for computing solutions for $\omega$ belonging to other intervals by considering $\omega^2 = \omega_0^2 - \Lambda$ where $-1/2 < \text{Im} \omega_0 < 0$ and $\text{Re} \omega_0 = 0$, and the equation is written in the form $-u'' + (q(x) + \Lambda) u = \omega_0^2 u$. For example, we tested this simple idea considering $\omega_0 = -i/4$ and $\Lambda = 100$, computing thus a solution for Example 10 with $\omega^2 = -100.0625$. Again already with $N = 30$ the value of both the absolute and the relative errors of the solution was of order $10^{-16}$.

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