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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 $-u''+q(x)u=\omega^2u$ is obtained in the form of a series possessing the following attractive feature. The truncation error is ω-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

$$-u''+q(x)u=\omega^2u \tag{1}$$

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 $\omega\in\mathbb{R}$, $|u(\omega,x)-u_N(\omega,x)|\le\varepsilon_N(x)$, where ε_N is a nonnegative function independent of ω 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

$$u(0)=1,\qquad u'(0)=-i\omega$$

was considered in the form

$$u(\omega,x)=e^{-i\omega x}+\int_{-x}^{x}K(x,y)e^{-i\omega y}dy, \tag{2}$$

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

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representation of $u(\omega, x)$ in the form

$$u(\omega,x)=e^{-i\omega x}+\int_{-\infty}^{x}\mathbf{A}(x,y)e^{-i\omega y}dy \tag{3}$$

where the kernel $\mathbf{A}(x,\cdot)\in L_2(-\infty,x)$ is that arising in the scattering theory associated with (1), see, e.g., [1]. Since the integral in (3) is taken over a semi-infinite interval it is natural to look for $\mathbf{A}(x,\ \cdot)$ 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 ω-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 2017, 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

$$-u''+q(x)u=\omega^2u \tag{4}$$

on a finite interval $(0, d)$. We suppose that q is a real valued, measurable function. The solution of (4) satisfying the initial conditions

$$u(0)=1,\qquad u'(0)=-i\omega, \tag{5}$$

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 (4) 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 $\mathbf{A}(x,\cdot)\in L_2(-\infty,x)$ that

$$u(\omega,x)=e^{-i\omega x}+\int_{-\infty}^{x}\mathbf{A}(x,y)e^{-i\omega y}dy\qquad\text{for all }\omega. \tag{6}$$

This integral representation of $u(\omega, x)$ can be viewed as action of an operator of transmutation (transformation) with the kernel $\mathbf{A}(x, y)$ on the solution $e^{-i\omega x}$ of the elementary equation $-u''=\omega^2u$. The kernel $\mathbf{A}(x, y)$ here is an extension by zero of the kernel $K(x, y)$ from (2) onto $y\in(-\infty,-x)$.

Denote the operator in (6) by $A[v](x):=v(x)+\int_{-\infty}^{x}\mathbf{A}(x,y)v(y)dy$.

Note that (see, e.g., [1])

$$\mathbf{A}(x,x)=\frac{1}{2}\int_0^x q(y)dy. \tag{7}$$

By a change of the integration variable equality (6) can be written as follows

$$u(\omega,x)=e^{-i\omega x}\left(1+\int_0^{\infty}\mathbf{A}(x,x-t)e^{i\omega t}dt\right).$$

Let us represent the kernel $\mathbf{A}(x,x-t)$ in the form $\mathbf{A}(x,x-t)=\mathbf{a}(x,t)e^{-t}$. The function $\mathbf{a}(x,\ \cdot)$ then belongs to the space $L_2\left(0,\infty;e^{-t}\right)$ equipped with the scalar product $\langle u,v\rangle:=\int_0^\infty u(t)\overline{v}(t)e^{-t}dt$ and the norm $\|u\|:=\sqrt{\langle u,u\rangle}$. Thus, for any $x\in[0, d]$ the function $\mathbf{a}(x,\ \cdot)$ admits a Fourier–Laguerre expansion convergent in this norm,

$$\mathbf{a}(x,t)=\sum_{n=0}^{\infty}a_n(x)L_n(t),$$

where L_n stands for the Laguerre polynomial of order n, and hence

$$\mathbf{A}(x,y)=\sum_{n=0}^{\infty}a_n(x)L_n(x-y)e^{-(x-y)}. \tag{8}$$