A single step second order of accuracy difference scheme for integral type nonlocal boundary value Schrödinger problem

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Abstract

In this study, nonlocal boundary value Schrödinger type problem in a Hilbert space with the self-adjoint operator is investigated. Single step stable second order of accuracy difference scheme for the numerical solution of this problem is presented. The main theorem on the stability of this difference scheme is established. Numerical results are given.

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1 Introduction

It is known that various problems in physics lead local and nonlocal boundary value problems to Schrödinger equations. Methods of solutions of the problems for Schrödinger have been studied extensively by many researchers (see e.g., [1, 2, 3, 4, 5, 6] and the references given therein). However, single step second order of accuracy difference scheme for nonlocal problems of Schrödinger equations have not been well-investigated so far. In the present paper the integral type nonlocal boundary value problem

$$\begin{cases} i\frac{du}{dt} + Au = f(t),\ 0 < t < T, \\ u(0) = \int\limits_0^T \alpha(s)u(s)ds + \varphi \end{cases} \tag{1.1}$$

for Schrödinger problem in a Hilbert space H with the self-adjoint operator A is considered. This problem was also considered in the article [6]. But in [6], to obtain approximate solution of this problem, first order accuracy Rothe difference scheme and second order accuracy Crank-Nicholson difference scheme are considered. On the other hand, in this study, single step stable second order of accuracy difference scheme for the numerical solution of this problem is presented. The main theorem on the stability of this difference scheme is established. A procedure of modified Gauss elimination method is used for solving this difference scheme. The method is illustrated by a numerical example.

2 A single step stable difference scheme

An integral type nonlocal boundary Schrödinger problem (1.1) is a well-posed problem. This fact follows from the following theorem.

Theorem 2.1. Assume that

$$\int_0^T |\alpha(s)|\, ds < 1.$$

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Then there exists a unique solution $u(t)$ of the problem (1.1) and the following inequalities are satisfied:

$$\max_{0\le t\le T}\|u(t)\|_H \le (1+C_\alpha)\left[\|\varphi\|_H + T\max_{0\le t\le T}\|f(t)\|_H\right] \tag{2.1}$$

and

$$\max_{0\le t\le T}\|u'(t)\|_H + \max_{0\le t\le T}\|Au(t)\|_H$$
$$\le (1+C_\alpha)\left[\|A\varphi\|_H + T\max_{0\le t\le T}\|f'(t)\|_H + \|f(0)\|_H\right] \tag{2.2}$$

where C_α denotes a positive constant depends on α and not depends on f and φ.

Th proof of this theorem is given in [5]. In order to obtain a single step second order stable difference scheme to obtain an approximate solution for an integral type nonlocal Schrödinger problem (1.1), we follow the book [7]. First of all let's state and prove the following auxiliary lemma.

Lemma 2.2. Let the function $v(t)$, $0 \le t \le T$ has a third order continuous derivative and $t_{k-1}, t_k \in [0,T]$. Then the following relation holds.

$$v(t_k) - v(t_{k-1}) - \frac{\tau}{2}v'(t_k) - \frac{\tau}{2}v'(t_{k-1})$$
$$= -\frac{1}{2}\int_{t_{k-1}}^{t_k}(t_k - s)(s - t_{k-1})v^{(3)}(s)ds. \tag{2.3}$$

Proof. Using the formula of integration by parts, we obtain the representation

$$\int_{t_{k-1}}^{t_k} w(s)v^{(3)}(s)ds$$
$$= (w(s)v'' - w'(s)v' + w''(s)v(s)|_{t_{k-1}}^{t_k} - \int_{t_{k-1}}^{t_k} w^{(3)}(s)v(s)ds. \tag{2.4}$$

If we take $w(s) = (t_k - s)(s - t_{k-1})^2$ then $w(t_k) = 0$, $wt_{k-1} = 0$, $w'(t_k) = -\tau$, $w't_{k-1} = \tau$, $w''(t_k) = -2$, $w't_{k-1} = -2$, and $w^{(3)}(s) = 0$. If we substitute these results into equation (2.4) and divide both sides by 6 we obtain the identity (2.3) . Q.E.D.

Note that the relation (2.3) is called the Taylor's decomposition of function $v(t)$ on two points. Now we wil consider the applications of the Taylor's decomposition of function on two points. From (2.3) it is clear that for the approximate solution of the problem (1.1) it is necessary to find $v'(t_k)$ and $v'(t_{k-1})$. Substituting the expression

$$v'(t) = iAv(t) - if(t) \tag{2.5}$$

in (2.3) and neglecting the expression of integral we obtain the single step difference schemes of second order of accuracy for the solution of equation $i\frac{du}{dt} + Au(t) = f(t)$. But for the approximation of integral in the integral type nonlocal boundary condition $u(0) = \int_0^T \alpha(s)u(s)ds + \varphi$, we use trapezoidal rule for the approximation of Riemann's integral since trapezoidal rule gives us a second order of approximation under smooth data. Hence for the approximate solution of the problem (1.1) we obtain the single step second order of accuracy difference scheme

$$\begin{cases} i\frac{u_k-u_{k-1}}{\tau}+A\left(\frac{u_k+u_{k-1}}{2}\right)=\varphi_k, \\ \varphi_k=\frac{1}{2}(f(t_k)+f(t_{k-1})) \\ t_k=k\tau, 1\le k\le N, N\tau=T, \\ u_0=\frac{\tau}{2}\left[\alpha(0)u(0)+\alpha(T)u(T)+2\sum\limits_{j=1}^{N-1}\alpha(t_j)u_j+\varphi\right] \end{cases} \tag{2.6}$$

generated by Taylor's decomposition on two points.
Now let us obtain a formula for the solution of (2.6). By induction

$$u_k=R^k\xi-i\tau\sum_{j=1}^{k}R^{k-j}P\varphi_j, 1\le k\le N \tag{2.7}$$

is the solution of the second order difference scheme

$$i\frac{u_k-u_{k-1}}{\tau}+A\left(\frac{u_k+u_{k-1}}{2}\right)=\varphi_k,\ 1\le k\le N,\ u_0=\xi \tag{2.8}$$

for the approximate solutions of the Cauchy problem

$$i\frac{du}{dt}+Au(t)=f(t), \qquad 0<t<T, \quad u(0)=\xi. \tag{2.9}$$

Here

$$R=\left(I+i\frac{\tau}{2}A\right)P \text{ and } P=\left(I-i\frac{\tau}{2}A\right)^{-1}. \tag{2.10}$$

Using formula (2.7) and the condition

$$u_0=\frac{\tau}{2}\left[\alpha(0)u(0)+\alpha(T)u(T)+2\sum_{j=1}^{N-1}\alpha(t_j)u_j+\varphi\right], \tag{2.11}$$

we get

$$\begin{aligned} u_0=\frac{\tau}{2}\Big[&\alpha(0)\xi+\alpha(T)(R^N\xi-i\tau\textstyle\sum_{m=1}^{N}R^{N-m}P\varphi_m) \\ &+2\sum_{j=1}^{N-1}\alpha(t_j)\left(R^j\xi-i\tau\textstyle\sum_{m=1}^{j}R^{j-m}P\varphi_m\right)+\varphi\Big]. \end{aligned} \tag{2.12}$$

Since the operator

$$I-\frac{\tau}{2}\left(\alpha(0)+\alpha(T)R^N+2\sum_{j=1}^{N-1}\alpha(t_j)R^j\right)$$

has an inverse, we obtain

$$\xi = \frac{\tau}{2} T_\tau \left[-i\tau\alpha(T) \sum_{m=1}^{N} R^{N-m} P\varphi_m) - 2i\tau \sum_{j=1}^{N-1} \sum_{m=1}^{j} \alpha(t_j) R^{j-m} P\varphi_m + \varphi \right] \tag{2.13}$$

where

$$T_\tau = \left(I - \frac{\tau}{2} \left(\alpha(0) + \alpha(T)R^N + 2\sum_{j=1}^{N-1} \alpha(t_j) R^j \right) \right)^{-1}. \tag{2.14}$$

So, for the solution of problem (2.6), we have the following formula:

$$u_k = \begin{cases} R^k \xi - i\tau \sum_{j=1}^{k} R^{k-j} P\varphi_j, \ 1 \le k \le N, \\ \frac{T_\tau \tau}{2} \left[-i\tau\alpha(T) \sum_{m=1}^{N} R^{N-m} P\varphi_m - 2i\tau \sum_{j=1}^{N-1} \sum_{m=1}^{j} \alpha(t_j) R^{j-m} P\varphi_m \right. \\ \left. +\varphi \right], \ k = 0. \end{cases} \tag{2.15}$$

Theorem 2.3. Assume that $T \max_{\le t \le T} |\alpha(t)|_H < 1$, then the solution of difference scheme (2.6) satisfies the stability inequality

$$\max_{0 \le k \le N} \|u_k\|_H \le (C_\alpha + 1) \left[\|\varphi\|_H + T \max_{1 \le t \le N} |\varphi_k|_H \right], \tag{2.16}$$

where C_α denotes a positive constant depends on α and not depends on τ, φ, φ_k.

Proof. Using the estimate

$$\|R\|_{H \to H} \le 1, \ \ \|P\|_{H \to H} \le 1 \tag{2.17}$$

and the formula (2.7), we can obtain

$$\max_{1 \le k \le N} \|u_k\|_H \le \left[\|u_0\|_H + T \max_{1 \le t \le N} |\varphi_k|_H \right]. \tag{2.18}$$

Using the spectral representation of self-adjoint operators one can establish

$$\|T_\tau\|_{H \to H} \le C_\alpha. \tag{2.19}$$

Namely,

$$\|T_\tau\|_{H \to H}$$

$$\le \sup_{-\infty \le \mu \le \infty} \left| \left(1 - \frac{\tau}{2} \left(\alpha(0) + \alpha(T)R^N + 2\sum_{j=1}^{N-1} \alpha(t_j) R^j \right) \right)^{-1} \right| \tag{2.20}$$

$$\leq \sup_{-\infty\leq\mu\leq\infty}\left|\frac{1}{1-\frac{\tau}{2}\left|\alpha(0)+\alpha(T)R^N+2\sum\limits_{j=1}^{N-1}\alpha(t_j)R^j\right|}\right| \tag{2.21}$$

Since

$$\frac{\tau}{3}\left|\alpha(0)+\alpha(T)R^N+2\sum_{j=1}^{N-1}\alpha(t_j)R^j\right| \tag{2.22}$$

$$\leq \frac{\tau}{2}\left(|\alpha(0)|_H+|\alpha(T)|_H+2\sum_{j=1}^{N-1}|\alpha(t_j)|_H\right) \tag{2.23}$$

$$\leq \frac{\tau}{2}2N\max_{0\leq t\leq T}|\alpha(t)|_H = T\max_{0\leq t\leq T}|\alpha(t)|_H<1, \tag{2.24}$$

we have that

$$\|T_\tau\|_{H\to H}\leq C_\alpha. \tag{2.25}$$

Then using formula (2.13), the triangle inequality and estimates (2.17) and (2.19) the following estimate is obtained:

$$\|u_0\|_H\leq C_\alpha\left[T\max_{1\leq k\leq N}\|\varphi_k\|+\|\varphi\|\right]. \tag{2.26}$$

Estimate (2.16) follows from (2.18) and (2.26). Q.E.D.

3 Numerical analysis

In this section, the numerical solutions of the integral type nonlocal boundary value

$$\begin{cases} i\frac{\partial u(t,x)}{\partial t}-\frac{\partial^2 u(t,x)}{\partial x^2}+u(t,x)=\exp(it\pi^2)\sin\pi x,\ 0<t,x<1, \\ u(0,x)=\frac{1}{10}\int\limits_0^1 u(s,x)ds+\varphi(x), \\ \varphi(x)=\left[-\frac{1}{10i\pi^2}\left(\exp i\pi^2-1\right)+1\right]\sin\pi x,\quad 0\leq x\leq 1, \\ u(t,0)=u(t,1)=0,\ 0\leq t\leq 1 \end{cases} \tag{3.1}$$

Schrödinger problem by using difference scheme (2.6) is investigated. The exact solution of this problem is

$$u\left(t,x\right)=\exp(it\pi^2)\sin\pi x.$$

For the approximate solution of problem (3.1), the set $[0,1]_\tau\times[0,1]_h$ of a family of grid points depending on the small parameters τ and h

$$\begin{aligned} [0,1]_\tau\times[0,1]_h &= \{(t_k,x_n): t_k=k\tau,\ \ 1\leq k\leq N-1,\ \ N\tau=1, \\ x_n &= nh,\ \ 1\leq n\leq M-1, Mh=1\} \end{aligned}$$

is defined. Applying (2.6) for the approximate solution of the problem (3.1), we get the following single step second order of accuracy difference scheme

$$\begin{cases} i\frac{u_n^k-u_n^{k-1}}{\tau}+\frac{1}{2}\left(-\frac{u_{n+1}^k-2u_n^k+u_{n-1}^k}{h^2}+u_n^k-\frac{u_{n+1}^{k-1}-2u_n^{k-1}+u_{n-1}^{k-1}}{h^2}+u_n^{k-1}\right) \\ =f(t_k,x_n),\quad 1\le k\le N-1,\ 1\le n\le M-1, \\ f(t_k,x_n)=\frac{1}{2}\left(\exp(it_k\pi^2)\sin\pi x_n+\frac{1}{3}\exp(it_{k-1}\pi^2)\right)\sin\pi x_n \\ u_n^0=\frac{\tau}{20}\left[u_n^0+u_n^M+2\sum\limits_{j=1}^{N-1}u_n^j\right]+\varphi(x_n),\ 1\le n\le M-1, \\ u_0^k=0,\ u_M^k=0,\ 0\le k\le N. \end{cases} \tag{3.2}$$

So we have $(M+1)\times(M+1)$ system of linear equations which can be written in the matrix form as:

$$\begin{cases} A\,U_{n+1}+BU_n+CU_{n-1}=D\varphi_n,\quad 1\le n\le M-1, \\ U_0=0,\ U_M=0, \end{cases} \tag{3.3}$$

where

$$\varphi_n=\begin{bmatrix}\varphi_n^0\\ \varphi_n^1\\ \cdots\\ \varphi_n^N\end{bmatrix}_{(N+1)\times 1},\quad \varphi_n^k=\begin{cases}\left[-\frac{1}{10i\pi^2}(\exp i\pi^2-1)+1\right](\sin\pi x_n),\ k=0,\\ f(t_k,x_n),\qquad 1\le k\le N,\end{cases}$$

$A(i,i)=A(i,i+1)=a$, $B(i,i)=b$, $B(i,i+1)=c$ for any $1\le i\le N$ and $B(N+1,1)=1-\tau/20$, $B(N+1,N+1)=-\tau/20$, $B(N+1,i)=-\tau/20$ for any $2\le i\le N$ and the other entries for the matrices A, B are all zero. The matrix D is an identity matrix of order $N+1$ and the matrix C is equal to the matrix A. In these matrices entries are given as:

$$a=-\frac{1}{2h^2},\ b=-\frac{i}{\tau}+\frac{1}{h^2}+\frac{1}{2},\ c=\frac{i}{\tau}+\frac{1}{h^2}+\frac{1}{2},$$

$$U_s=\begin{bmatrix}U_s^0\\ U_s^1\\ \cdots\\ U_s^{N-1}\\ U_s^N\end{bmatrix},\quad s=\ n-1,n,n+1.$$

Thus, we have the single step second order difference equations with respect to n with matrix coefficients. To solve these difference equation we have applied the same modified Gauss elimination method as in [6] for the difference equation with respect to n with matrix coefficients. Hence, we seek a solution of the matrix in the following form

$$U_n=\alpha_{n+1}U_{n+1}+\beta_{n+1},\qquad n=M-2,...,2,1,0, \tag{3.4}$$

where α_j $(j = 1, ..., M)$ are $(N+1)\times(N+1)$ square matrices and β_j $(j = 1, ..., M)$ are $(N+1)\times 1$ column matrices. defined by

$$\alpha_{n+1} = -\left(B + C\alpha_n\right)^{-1} A, \quad \beta_{n+1} = \left(B + C\alpha_n\right)^{-1}\left(D\varphi_n - C\beta_n\right), \tag{3.5}$$

$n = 1, 2, 3, \cdot\cdot\cdot, M-1$.
Then using formulas (3.4) and (3.1), we can compute U_n, $0 \le n \le M$.
For their comparison, the errors computed by

$$E = \max_{\substack{1\le k\le N \\ 1\le n\le M}} \left|u(t_k, x_n) - u_n^k\right|.$$

Tables 1 gives the error analysis between the exact solution and the solutions derived by difference schemes. Table 1 is constructed for $N = M = 20$, 40, 80 and 160 respectively.

Table 1
Comparison of the errors for the approximate solution of problem (3.1).

Method	N=M=20	N=M=40	N=M=80	N=M=160
Single Step Second Order	0.1378	0.0360	0.0091	0.0023
Crack-Nicholson	0.1569	0.0410	0.0104	0.0026

Second, for their comparison, the relative errors are computed by

$$relE_N^M = \max_{1\le k\le N} \frac{E_N^M}{\left(\sum_{n=1}^{M} \left|u(t_k, x_n)\right|^2 h\right)^{\frac{1}{2}}}$$

and the Table 2 is constructed for $N = M = 20$, 40, 80 and 160 respectively.

Table 2
Comparison of the relative errors for the approximate solution of problem (3.1).

Method	N=M=20	N=M=40	N=M=80	N=M=160
Single Step Second Order	0.1949	0.0509	0.0129	0.0033
Crack-Nicholson	0.2218	0.0579	0.0147	0.0037

In this research, to obtain an approximate solution for an integral type nonlocal boundary value Schrödinger problem, a single step stable second order difference scheme is established. The stability of this difference scheme is proved. Even if this difference scheme is easy to implement, it is seen from the tables that it gives same good approximation with Crank-Nicholson difference scheme for integral type nonlocal boundary Schrödinger problem.

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