Research Article

Modified Crank-Nicolson Difference Schemes for Nonlocal Boundary Value Problem for the Schrödinger Equation

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The nonlocal boundary value problem for Schrödinger equation in a Hilbert space is considered. The second-order of accuracy r -modified Crank-Nicolson difference schemes for the approximate solutions of this nonlocal boundary value problem are presented. The stability of these difference schemes is established. A numerical method is proposed for solving a one-dimensional nonlocal boundary value problem for the Schrödinger equation with Dirichlet boundary condition. A procedure of modified Gauss elimination method is used for solving these difference schemes. The method is illustrated by numerical examples.

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1. Introduction

In this article, the nonlocal boundary value problem for the Schrödinger equation

$$\begin{aligned}iu'(t) + Au(t) &= f(t), \quad 0 < t < T, \\u(0) &= \sum_{m=1}^p \alpha_m u(\lambda_m) + \varphi, \\0 < \lambda_1 < \lambda_2 < \dots < \lambda_p &\leq T\end{aligned}\tag{1.1}$$

in a Hilbert space H with the self-adjoint operator A is considered. The Schrödinger equation plays an important role in the modeling of many phenomena. Methods of solutions for the

Schrödinger equation have been studied extensively by many researchers (see, e.g., [1–9] and the references given therein).

The idea in this work is inspired from the works [2, 3, 10, 11]. In the articles [2, 3] the existence and the uniqueness of the solution of the nonlocal boundary value problem (1.1) and its general form under some conditions are studied. In the article [8], to find an approximate solution of the problem (1.1), first-order of accuracy Rothe difference scheme and second-order of accuracy Crank-Nicolson difference scheme are presented. The stability estimates for the solution of this problem and the stability of these difference schemes are established.

The main aim of this paper is to study r modified Crank-Nicolson difference schemes for the approximate solution of problem (1.1). The paper is organized as follows. In Section 2, we establish estimates for the stability of higher order derivatives of the solution of problem (1.1). In Section 3, the second-order of accuracy r modified Crank-Nicolson difference schemes for the approximate solution of problem (1.1) are presented. The stabilities of these difference schemes are established. In Section 4, we study the convergence of these difference schemes. In Section 5, a numerical example is exposed in order to validate the schemes. A procedure involving the modified Gauss elimination method is used for solving these difference schemes.

Throughout this paper, the constants used are not necessarily the same at different occurrences.

2. Nonlocal Boundary Value Problem

Theorem 2.1. *Assume that $f(t) \in C^1([0, T], H)$, $\varphi \in D(A)$ and*

$$\sum_{m=1}^p |\alpha_m| < 1. \quad (2.1)$$

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

$$\max_{0 \leq t \leq T} \|u(t)\|_H \leq C(\alpha_1, \dots, \alpha_p) \left[\|\varphi\|_H + T \max_{0 \leq t \leq T} \|f(t)\|_H \right], \quad (2.2)$$

$$\begin{aligned} & \max_{0 \leq t \leq T} \|u'(t)\|_H + \max_{0 \leq t \leq T} \|Au(t)\|_H \\ & \leq C(\alpha_1, \dots, \alpha_p) \left[\|A\varphi\|_H + T \max_{0 \leq t \leq T} \|f'(t)\|_H + \|f(0)\|_H \right]. \end{aligned} \quad (2.3)$$

Proof. The proof of the estimate (2.2) is given in [8]. Now we will obtain the estimate (2.3).

It is known that for smooth data of the problem

$$iu'(t) + Au(t) = f(t), \quad 0 < t < T, \quad u(0) = \xi, \quad (2.4)$$

there exists a unique solution of the problem (1.1), and the following formula holds:

$$u(t) = e^{iAt}\xi - \int_0^t e^{iA(t-s)}if(s)ds. \quad (2.5)$$

Therefore we have

$$Au(t) = e^{iAt}A\xi + f(0) + \int_0^t f'(s)ds - f(0)e^{iAt} - \int_0^t e^{iA(t-s)}f'(s)ds. \quad (2.6)$$

So that we get the estimate

$$\max_{0 \leq t \leq T} \|u(t)\|_H \leq \|A\xi\|_H + 2\|f(0)\|_H + 2T \max_{0 \leq t \leq T} \|f'(t)\|_H. \quad (2.7)$$

Using the condition $u(0) = \sum_{m=1}^p \alpha_m u(\lambda_m) + \varphi$ and the formula (2.6) we get

$$\begin{aligned} A\xi = R \left\{ \sum_{m=1}^p \alpha_m f(0) + \sum_{m=1}^p \alpha_m \int_0^{\lambda_m} f'(s)ds - f(0) \sum_{m=1}^p \alpha_m e^{iA\lambda_m} \right. \\ \left. - \sum_{m=1}^p \alpha_m \int_0^{\lambda_m} e^{iA(\lambda_m-s)} f'(s)ds + A\varphi \right\}, \end{aligned} \quad (2.8)$$

where

$$R = \left(I - \sum_{m=1}^p \alpha_m e^{iA\lambda_m} \right)^{-1}. \quad (2.9)$$

By using estimates

$$\|R\|_{H \rightarrow H} \leq \frac{1}{1 - \sum_{m=1}^p |\alpha_m|} \leq C(\alpha_1, \dots, \alpha_p), \quad \|e^{iAt}\|_{H \rightarrow H} \leq 1, \quad (2.10)$$

and the assumption $\sum_{m=1}^p |\alpha_m| < 1$, we get

$$\|A\xi\|_H \leq C(\alpha_1, \dots, \alpha_p) \left\{ 2\|f(0)\|_H + 2T \max_{0 \leq t \leq T} \|f'(t)\|_H + \|A\varphi\|_H \right\}. \quad (2.11)$$

By using the estimates (2.7) and (2.11) we obtain an estimate for Au . Then by using the estimate for Au , the relation $iu'(t) = f(t) - Au = f(0) + \int_0^t f'(s)ds - Au$ and the triangle inequality we can obtain estimate (2.3). This completes the proof of Theorem 2.1. $\square$

3. Difference Schemes, Stability

In this section, we present r -modified Crank-Nicolson difference schemes for the approximate solutions of problem (1.1) and establish the stabilities of these difference schemes. It is assumed that $2\tau \leq \lambda_m$ for $1 \leq m \leq p$. Let us associate the nonlocal boundary value problem (1.1) with the corresponding second-order of accuracy r -modified Crank-Nicolson difference schemes:

$$\begin{aligned} i \frac{u_k - u_{k-1}}{\tau} + \frac{A}{2}(u_k + u_{k-1}) &= \varphi_k, \quad r+1 \leq k \leq N, \\ i \frac{u_k - u_{k-1}}{\tau} + Au_k &= \varphi_k, \quad 1 \leq k \leq r, \\ u_0 &= \sum_{r\tau \geq \lambda_m} \alpha_m ((I + il_{0m}A)u_{lm} - il_{0m}\varphi_{lm}) + \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \in Z^+}} \alpha_m u_{lm} \\ &+ \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin Z^+}} \alpha_m (I + id_m A) \frac{1}{2}(u_{lm} + u_{lm+1}) - i \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin Z^+}} \alpha_m d_m \varphi_{lm} + \varphi, \\ 0 < \lambda_1 < \lambda_2 < \dots < \lambda_p &\leq T, \end{aligned} \quad (3.1)$$

for the approximate solutions of this nonlocal boundary value problem. Z^+ denotes here the set $\{2, \dots, n, \dots\}$ and $l_m = \lfloor \lambda_m/\tau \rfloor$, $l_{0m} = \lambda_m - \lfloor \lambda_m/\tau \rfloor \tau$, $d_m = \lambda_m - \lfloor \lambda_m/\tau \rfloor \tau - \tau/2$, $\varphi_k = f(t_k - \tau/2)$, $t_k = k\tau$, where $\lfloor x \rfloor$ stands for the greatest integer part of the real number x .

By [10],

$$u_k = \begin{cases} R^k \xi - i\tau \sum_{j=1}^k R^{k-j+1} \varphi_j, & k = 1, \dots, r, \\ B^{k-r} R^r \xi - i\tau \sum_{j=1}^r B^{k-r} R^{r-j+1} \varphi_j - i\tau \sum_{j=r+1}^k B^{k-j} C \varphi_j, & k = r+1, \dots, N \end{cases} \quad (3.2)$$

is the solution of the r -modified Crank-Nicolson difference schemes for the approximate solutions of Cauchy problem

$$\begin{aligned} i \frac{u_k - u_{k-1}}{\tau} + \frac{A}{2}(u_k + u_{k-1}) &= \varphi_k, \quad r+1 \leq k \leq N, \\ i \frac{u_k - u_{k-1}}{\tau} + Au_k &= \varphi_k, \quad 1 \leq k \leq r, \quad u_0 = \xi. \end{aligned} \quad (3.3)$$

Here

$$R = (I - i\tau A)^{-1}, \quad C = \left(I - i\frac{A}{2}\tau\right)^{-1}, \quad B = \left(I + i\frac{A}{2}\tau\right)C. \quad (3.4)$$

For u_0 , using the formula (3.2) and the condition we obtain

$$\begin{aligned} \xi = T_\tau \Bigg\{ & \left(-i\tau \sum_{r\tau \geq \lambda_m} \alpha_m (I + il_{0m}A) \sum_{j=1}^{l_m} R^{l_m-j+1} \varphi_j - i \sum_{r\tau \geq \lambda_m} \alpha_m l_{0m} \varphi_{lm} \right) \\ & - i\tau \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \in Z^+}} \alpha_m \left(\sum_{j=1}^r B^{l_m-r} R^{r-j+1} \varphi_j + \sum_{j=r+1}^{l_m} B^{l_m-j} C \varphi_j \right) \\ & - i\tau \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin Z^+}} \alpha_m (I + id_m A) \frac{1}{2} \left((I + B) \left(\sum_{j=1}^r B^{l_m-r} R^{r-j+1} \varphi_j + \sum_{j=r+1}^{l_m} B^{l_m-j} C \varphi_j \right) + C \varphi_{l_m+1} \right) \\ & \left. - i \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin Z^+}} \alpha_m d_m A + \varphi \right\}, \end{aligned} \quad (3.5)$$

where

$$\begin{aligned} T_\tau = & \left(I - \sum_{r\tau \geq \lambda_m} \alpha_m (I + il_{0m}A) R^{l_m} - \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \in Z^+}} \alpha_m B^{l_m-r} R^r \right. \\ & \left. - \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin Z^+}} \alpha_m (I + id_m A) \frac{1}{2} (I + B) B^{l_m-r} R^r \right)^{-1}. \end{aligned} \quad (3.6)$$

Note that, here we considered $\sum_{k=r+1}^{l_m} B^{l_m-j} C \varphi_j = 0$ for $l_m = r$. So, for the solution of problem (3.2), we have the following formula:

$$u_k = \begin{cases} R^k u_0 - i\tau \sum_{j=1}^k R^{k-j+1} \varphi_j, & k = 1, \dots, r, \\ B^{k-r} R^r u_0 - i\tau \sum_{j=1}^r B^{k-r} R^{r-j+1} \varphi_j - i\tau \sum_{j=r+1}^k B^{k-j} C \varphi_j, & k = r+1, \dots, N, \\ T_\tau \left\{ \begin{aligned} & -i\tau \sum_{r\tau \geq \lambda_m} \alpha_m (I + i l_{0m} A) \sum_{j=1}^{l_m} R^{l_m-j+1} \varphi_j - i \sum_{r\tau \geq \lambda_m} \alpha_m l_{0m} \varphi_{l_m} \\ & -i\tau \sum_{\substack{r\tau < \lambda_m \\ \lambda/\tau \in \mathbb{Z}^+}} \alpha_m \left(\sum_{j=1}^r B^{l_m-r} R^{r-j+1} \varphi_j + \sum_{j=r+1}^{l_m} B^{l_m-j} C \varphi_j \right) \\ & -i\tau \sum_{\substack{r\tau < \lambda_m \\ \lambda/\tau \notin \mathbb{Z}^+}} \alpha_m (I + i d_m A) \\ & \times \frac{1}{2} \left((I + B) \left(\sum_{j=1}^r B^{l_m-r} R^{r-j+1} \varphi_j + \sum_{j=r+1}^{l_m} B^{l_m-j} C \varphi_j \right) + C \varphi_{l_m+1} \right) \\ & -i \sum_{\substack{r\tau < \lambda_m \\ \lambda/\tau \notin \mathbb{Z}^+}} \alpha_m d_m \varphi_{l_m} + \varphi \end{aligned} \right\}, & k = 0. \end{cases} \quad (3.7)$$

Theorem 3.1. Assume that $\varphi \in D(A)$ and

$$\sum_{m=1}^p |\alpha_m| < 1. \quad (3.8)$$

Then the solutions of the difference schemes (3.1) satisfy the stability inequalities

$$\max_{0 \leq k \leq N} \|u_k\|_H \leq C(\alpha_1, \dots, \alpha_p) \left[\|\varphi\|_H + T \max_{1 \leq k \leq N} \|\varphi_k\|_H \right], \quad (3.9)$$

$$\begin{aligned} & \max_{1 \leq k \leq N} \left\| \frac{u_k - u_{k-1}}{\tau} \right\|_H + \max_{1 \leq k \leq r} \|A u_k\|_H + \max_{r+1 \leq k \leq N} \left\| A \frac{u_k + u_{k-1}}{2} \right\|_H \\ & \leq C(\alpha_1, \dots, \alpha_p) \left[\|A \varphi\|_H + \|\varphi_1\|_H T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H \right]. \end{aligned} \quad (3.10)$$

Proof. Using the estimates

$$\|R\|_{H \rightarrow H} \leq 1, \quad \|B\|_{H \rightarrow H} \leq 1, \quad \|C\|_{H \rightarrow H} \leq 1, \quad (3.11)$$

and the formula (3.2), we can obtain

$$\max_{1 \leq k \leq N} \|u_k\|_H \leq \left[\|u_0\|_H + T \max_{1 \leq k \leq N} \|\varphi_k\|_H \right]. \quad (3.12)$$

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

$$\|T_\tau\|_{H \rightarrow H} \leq \frac{1}{1 - \sum_{m=1}^p |\alpha_m|} \leq C(\alpha_1, \dots, \alpha_p). \quad (3.13)$$

Estimate for $\|u_0\|_H$ should also be examined. By using formula (3.7), the triangle inequality, and estimates (3.11), (3.13) the following estimate is obtained:

$$\|u_0\|_H \leq C(\alpha_1, \dots, \alpha_p) \left[\|\varphi\|_H + 2T \max_{1 \leq k \leq N} \|\varphi_k\|_H \right]. \quad (3.14)$$

The proof of the estimate (3.9) for the difference schemes (3.1) is based on the last estimate and estimate (3.12).

Now, estimate (3.10) will be obtained. Using (3.2), we get

$$Au_k = \begin{cases} R^k A\xi - i\tau \sum_{j=1}^k AR^{k-j+1}\varphi_j, & k = 1, \dots, r, \\ B^{k-r} R^r A\xi - i\tau \sum_{j=1}^r B^{k-r} AR^{r-j+1}\varphi_j - i\tau \sum_{j=r+1}^k B^{k-j} AC\varphi_j, & k = r+1, \dots, N. \end{cases} \quad (3.15)$$

So that

$$Au_k = \begin{cases} R^k A\xi + \left(\sum_{j=2}^k R^{k-j+1}(\varphi_{j-1} - \varphi_j) + \varphi_k - R^k \varphi_1 \right), & k = 1, \dots, r, \\ B^{k-r} R^r A\xi + \sum_{j=2}^r B^{k-r} R^{r-j+1}(\varphi_{j-1} - \varphi_j) - B^{k-r} R^r \varphi_1 \\ \quad + \sum_{j=r+1}^k B^{k-j+1}(\varphi_{j-1} - \varphi_j) + \varphi_k, & k = r+1, \dots, N. \end{cases} \quad (3.16)$$

For the estimate (3.10) the two cases should be examined separately: (i) $k = 1, \dots, r$, (ii) $k = r+1, \dots, N$. Let $1 \leq k \leq r$. Then, using (3.16) we get

$$\max_{1 \leq k \leq r} \|Au_k\|_H \leq \|RA\xi\|_H + 2N \max_{2 \leq k \leq N} \|\varphi_k - \varphi_{k-1}\|_H + 2\|\varphi_1\|_H. \quad (3.17)$$

Therefore,

$$\max_{1 \leq k \leq r} \|Au_k\|_H \leq \|RA\xi\|_H + 2T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H + 2\|\varphi_1\|_H. \quad (3.18)$$

Estimate for $\|RA\xi\|_H$ should also be obtained. Using the formula (3.5) and the formula (3.16) we get

$$\begin{aligned}
\xi = T_\tau \left\{ \sum_{r\tau \geq \lambda_m} \alpha_m (I + il_{0m}A) R \left(\sum_{j=2}^{l_m} R^{l_m-j+1} (\varphi_{j-1} - \varphi_j) + \varphi_{l_m} - R^{l_m} \varphi_1 \right) \right. \\
- i \sum_{r\tau \geq \lambda_m} \alpha_m l_{0m} RA \varphi_{l_m} + \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \in \mathbb{Z}^+}} \alpha_m R \left(\sum_{j=2}^r B^{l_m-r} R^{r-j+1} (\varphi_{j-1} - \varphi_j) - R^r \varphi_1 \right) \\
+ \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \in \mathbb{Z}^+}} \alpha_m R \left(\sum_{j=r+1}^{l_m} B^{l_m-j} C (\varphi_{j-1} - \varphi_j) + \varphi_{l_m} \right) + \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin \mathbb{Z}^+}} \alpha_m (I + id_m A) \\
\times \frac{1}{2} R \left(\left(\sum_{j=2}^r B^{l_m-r} R^{r-j+1} (\varphi_{j-1} - \varphi_j) - R^r \varphi_1 + \sum_{j=r+1}^{l_m} B^{l_m-j+1} (\varphi_{j-1} - \varphi_j) + \varphi_{l_m} \right) \right. \\
\left. + \left(\sum_{j=2}^r B^{l_m+1-r} R^{r-j+1} (\varphi_{j-1} - \varphi_j) - R^r \varphi_1 + \sum_{j=r+1}^{l_m+1} B^{l_m-j+2} (\varphi_{j-1} - \varphi_j) + \varphi_{l_m+1} \right) \right) \\
\left. - i \sum_{\substack{r\tau < \lambda_m \\ \lambda_m/\tau \notin \mathbb{Z}^+}} \alpha_m d_m AR \varphi_{l_m} + RA \varphi \right\}. \tag{3.19}
\end{aligned}$$

So that

$$\|RA\xi\|_H \leq C_1(\alpha_1, \dots, \alpha_p) \left[\|A\varphi\|_H + \|\varphi_1\|_H + T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H \right]. \tag{3.20}$$

Therefore, using the estimates (3.18) and (3.20) we obtain

$$\max_{1 \leq k \leq r} \|Au_k\|_H \leq C_2(\alpha_1, \dots, \alpha_p) \left[\|A\varphi\|_H + \|\varphi_1\|_H + T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H \right]. \tag{3.21}$$

Then using the estimate for Au_k , the relation $i((u_k - u_{k-1})/\tau) = \varphi_k - Au_k = \varphi_1 - \sum_{j=2}^k (\varphi_{j-1} - \varphi_j) - Au_k$, and the triangle inequality we get the estimate

$$\begin{aligned}
& \max_{1 \leq k \leq r} \left\| \frac{u_k - u_{k-1}}{\tau} \right\|_H + \max_{1 \leq k \leq r} \|Au_k\|_H \\
& \leq C_2(\alpha_1, \dots, \alpha_p) \left[\|A\varphi\|_H + \|\varphi_1\|_H + T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H \right]. \tag{3.22}
\end{aligned}$$

Now, let $k = r + 1, \dots, N$. Then using the formula (3.16) and the identity $(1/2)(I + B) = C$ we get

$$\begin{aligned} A \frac{u_k + u_{k-1}}{2} &= B^{k-r-1} C^{r-1} C R A \xi + \sum_{j=2}^r C B^{k-1-r} R^{r-j+1} (\varphi_{j-1} - \varphi_j) - R^r \varphi_1 \\ &+ \sum_{j=r+1}^k C B^{k-j} (\varphi_{j-1} - \varphi_j) + B(\varphi_{k-1} - \varphi_k) + \frac{\varphi_k + \varphi_{k-1}}{2}. \end{aligned} \quad (3.23)$$

So that

$$\max_{r+1 \leq k \leq N} \left\| A \frac{u_k + u_{k-1}}{2} \right\|_H \leq \|R A \xi\|_H + 3T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H + 3\|\varphi_1\|_H. \quad (3.24)$$

Therefore, using the estimates (3.20) and (3.24), the estimate

$$\max_{r+1 \leq k \leq N} \left\| A \frac{u_k + u_{k-1}}{2} \right\|_H \leq C_3(\alpha_1, \dots, \alpha_p) \left[\|A\varphi\|_H + \|\varphi_1\|_H + T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H \right] \quad (3.25)$$

is obtained. Then, by using the estimate (3.25), the relation $i((u_k - u_{k-1})/\tau) = \varphi_k - A((u_k + u_{k-1})/2) = \varphi_1 - \sum_{j=2}^k (\varphi_{j-1} - \varphi_j) - A((u_k + u_{k-1})/2)$, and the triangle inequality we get the estimate

$$\begin{aligned} \max_{r+1 \leq k \leq N} \left\| \frac{u_k - u_{k-1}}{\tau} \right\|_H &+ \max_{r+1 \leq k \leq N} \left\| A \frac{u_k + u_{k-1}}{2} \right\|_H \\ &\leq C_4(\alpha_1, \dots, \alpha_p) \left[\|A\varphi\|_H + \|\varphi_1\|_H + T \max_{2 \leq k \leq N} \left\| \frac{\varphi_k - \varphi_{k-1}}{\tau} \right\|_H \right]. \end{aligned} \quad (3.26)$$

The result (3.10) follows from the estimates (3.22) and (3.26). So the proof is complete. $\square$

4. Convergence

Theorem 4.1. Assume that $\sum_{m=1}^p |\alpha_m| < 1$. Assume also that $Au''(t)$ ($0 \leq t \leq T$) and $u'''(t)$ ($0 \leq t \leq T$) are continuous, then the solution of the difference scheme (3.1) satisfies the convergence estimate

$$\max_{0 \leq k \leq N} \|u_k - u(t_k)\|_H \leq M^*(r) \tau^2, \quad (4.1)$$

where $M^*(r)$ does not depend on τ but depends on r .

Proof. If we subtract (1.1) from (3.1) we obtain

$$\begin{aligned}
 i \frac{z_k - z_{k-1}}{\tau} + \frac{A}{2}(z_k + z_{k-1}) &= A_k, \quad r+1 \leq k \leq N, \\
 i \frac{z_k - z_{k-1}}{\tau} + A z_k &= A_k, \quad 1 \leq k \leq r, \\
 z_0 &= \sum_{r\tau \geq \lambda_m} \alpha_m ((I + i l_{0m} A) z_{lm} - i l_{0m} A_{lm}) + \sum_{\substack{r\tau < \lambda_m \\ \lambda_m / \tau \in \mathbb{Z}^+}} \alpha_m z_{lm} \\
 &+ \sum_{\substack{r\tau < \lambda_m \\ \lambda_m / \tau \notin \mathbb{Z}^+}} \alpha_m (I + i d_m A) \frac{1}{2} (z_{lm} + z_{lm+1}) - i \sum_{\substack{r\tau < \lambda_m \\ \lambda_m / \tau \notin \mathbb{Z}^+}} \alpha_m d_m A_{lm} + A_0, \\
 0 &< \lambda_1 < \lambda_2 < \dots < \lambda_p \leq T,
 \end{aligned} \tag{4.2}$$

where $z_k = u_k - u(t_k)$ and A_k is defined by the formula

$$A_k = \begin{cases} i \left(\frac{d}{dt} (u(t_{k-1/2})) - \frac{u(t_k) - u(t_{k-1})}{\tau} \right) + A(u(t_{k-1/2}) - u(t_k)), & 1 \leq k \leq r, \\ i \left(\frac{d}{dt} (u(t_{k-1/2})) - \frac{u(t_k) - u(t_{k-1})}{\tau} \right) + A \left(u(t_{k-1/2}) - \frac{u(t_k) + u(t_{k-1})}{2} \right), & r+1 \leq k \leq N, \\ \sum_{r\tau \geq \lambda_m} \alpha_m (I + i l_{0m} A) u(t_{lm}) + \sum_{\substack{r\tau < \lambda_m \\ \lambda_m / \tau \in \mathbb{Z}^+}} \alpha_m u(t_{lm}) \\ + \sum_{\substack{r\tau < \lambda_m \\ \lambda_m / \tau \notin \mathbb{Z}^+}} (I + i d_m A) \frac{1}{2} (u(t_{lm}) + u(t_{lm+1})) - \sum_{m=1}^p \alpha_m u(\lambda_m) \\ + i \sum_{r\tau \geq \lambda_m} \alpha_m l_{0m} (A_{lm} - \varphi_{lm}) + i \sum_{\substack{r\tau < \lambda_m \\ \lambda_m / \tau \notin \mathbb{Z}^+}} \alpha_m d_m (A_{lm} - \varphi_{lm}), & k = 0. \end{cases} \tag{4.3}$$

Then the difference problem (4.2) has a solution in the form (3.7), but instead of u_k, φ_k, φ we take $z_k, A_k, A_0, k = 1, \dots, N$, respectively. Using the estimates

$$\|R\|_{H \rightarrow H} \leq 1, \quad \|B\|_{H \rightarrow H} \leq 1, \quad \|C\|_{H \rightarrow H} \leq 1, \tag{4.4}$$

and the formula obtained for the solution of (4.2), we can obtain

$$\begin{aligned}
 \max_{1 \leq k \leq r} \|z_k\|_H &\leq \left[\|z_0\|_H + r\tau \max_{1 \leq k \leq r} \|A_k\|_H \right], \\
 \max_{r+1 \leq k \leq N} \|z_k\|_H &\leq \left[\|z_0\|_H + T \max_{1 \leq k \leq r} \|A_k\|_H \right].
 \end{aligned} \tag{4.5}$$

By the estimate (3.14) we have

$$\|z_0\|_H \leq C(\alpha_1, \dots, \alpha_p) \left[\|A_0\|_H + 2T \max_{1 \leq k \leq N} \|A_k\|_H \right]. \quad (4.6)$$

Therefore, in order to obtain the inequality (4.1) we need estimates for A_k for $0 \leq k \leq N$.

For $0 \leq k \leq N$, by the use of the triangle inequality, Taylor's formula, continuity of $Au''(t)$ ($0 \leq t \leq T$) and $u'''(t)$ ($0 \leq t \leq T$), the estimates

$$\max_{1 \leq k \leq r} \|A_k\|_H \leq M_1 \tau, \quad \max_{r+1 \leq k \leq N} \|A_k\|_H \leq M_2 \tau^2, \quad \|A_0\|_H \leq M_2 \tau^2 \quad (4.7)$$

are obtained. From the last estimates the result follows. $\square$

5. Numerical Results

In this section, the numerical experiments of the nonlocal boundary value problem

$$\begin{aligned} i \frac{\partial u(t, x)}{\partial t} - ((x+1)u_x)_x &= f(t, x), \quad 0 < t, x < 1, \\ u(0, x) &= \frac{1}{3} u\left(\frac{1}{2}, x\right) + \varphi(x), \quad 0 < x < 1, \\ u(t, 0) &= u(t, 1) = 0, \quad 0 < t < 1, \\ f(t, x) &= \left[\pi^2 \sin \pi x - \pi \cos \pi x + \pi^2 (x+1) \sin \pi x \right] \exp(-it), \\ \varphi(x) &= \left(1 - \frac{1}{3} \exp\left(-\frac{i}{2}\right) \right) (\sin \pi x). \end{aligned} \quad (5.1)$$

by using modified Crank-Nicolson difference scheme (3.1) are investigated. The exact solution of this problem is

$$u(t, x) = (\sin \pi x) \exp(-it). \quad (5.2)$$

For the approximate solution of problem (5.1), the set $[0, 1]_\tau \times [0, 1]_h$ of a family of grid points depending on the small parameters τ and h

$$[0, 1]_\tau \times [0, 1]_h = \{(t_k, x_n) : t_k = k\tau, 1 \leq k \leq N-1, N\tau = 1, x_n = nh, 1 \leq n \leq M-1, Mh = 1\} \quad (5.3)$$

is defined.

Applying the second-order of accuracy modified Crank-Nicolson difference schemes (3.1) we present following second-order of accuracy difference schemes for the approximate solutions of problem (5.1)

$$i \frac{u_n^k - u_n^{k-1}}{\tau} - \frac{1}{2} \left(\frac{u_{n+1}^k - u_{n-1}^k}{2h} + \frac{u_{n+1}^{k-1} - u_{n-1}^{k-1}}{2h} \right) - \frac{x_n + 1}{2} \left(\frac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{h^2} + \frac{u_{n+1}^{k-1} - 2u_n^{k-1} + u_{n-1}^{k-1}}{h^2} \right)$$

$$= f(t_{k-1/2}, x_n), \quad r+1 \leq k \leq N-1, 1 \leq n \leq M-1,$$

$$i \frac{u_n^k - u_n^{k-1}}{\tau} - \frac{u_{n+1}^k - u_{n-1}^k}{2h} - (x_n + 1) \frac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{h^2}$$

$$= f\left(t_k - \frac{\tau}{2}, x_n\right), \quad 1 \leq k \leq r, 1 \leq n \leq M-1,$$

$$t_{k-1/2} = \left(k - \frac{1}{2}\right)\tau, \quad x_n = nh, \quad 1 \leq k \leq N, 1 \leq n \leq M-1,$$

$$u_n^0 = \frac{1}{3} u_n^{[1/2\tau]} + \varphi(x_n), \quad 1 \leq n \leq M-1,$$

$$u_0^k = 0, \quad u_M^k = 0, \quad 0 \leq k \leq N.$$

(5.4)

So for each r , we have $(N+1) \times (N+1)$ system of linear equations which can be written in the matrix form as

$$A_n U_{n+1} + B_n U_n + C_n U_{n-1} = D_n \varphi_n, \quad 1 \leq n \leq M-1,$$

(5.5)

$$U_0 = 0, \quad U_M = 0,$$

where

$$\varphi_n = \begin{bmatrix} \varphi_n^0 \\ \varphi_n^1 \\ \dots \\ \varphi_n^N \end{bmatrix}_{(N+1) \times 1}, \quad \varphi_n^k = \begin{cases} \left(1 - \frac{1}{3} \exp\left(-\frac{i}{2}\right)\right) (\sin \pi x_n), & k = 0, \\ f(t_{k-1/2}, x_n), & 1 \leq k \leq N, \end{cases}$$

$$\begin{aligned}
A_n &= \begin{bmatrix} 0 & a_n & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & a_n & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & 0 & e_n & e_n & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & e_n & e_n & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & e_n & e_n \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \\
B_n &= \begin{bmatrix} b_n & c_n & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & b_n & c_n & \cdots & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & \cdots & \cdots & 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & \cdots & v_n & s_n & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & v_n & s_n & 0 \\ 0 & 0 & 0 & \cdots & 0 & \cdots & 0 & 0 & 0 & v_n & s_n \\ 1 & 0 & 0 & \cdots & -\frac{1}{3} & \cdots & 0 & 0 & 0 & 0 & 0 \end{bmatrix}, \\
C_n &= \begin{bmatrix} 0 & d_n & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & d_n & \cdots & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & g_n & g_n & 0 & 0 & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & 0 & g_n & g_n & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & g_n & g_n \\ 0 & 0 & 0 & \cdots & 0 & 0 & 0 & 0 & 0 \end{bmatrix},
\end{aligned}$$

$$D = I_{N+1}((N+1) \times (N+1) \text{ identity matrix}),$$

$$U_s = \begin{bmatrix} U_s^0 \\ U_s^1 \\ \cdots \\ U_s^{N-1} \\ U_s^N \end{bmatrix}, \quad s = n-1, n, n+1. \quad (5.6)$$

Table 1: Comparison of the errors for the approximate solution of problem (5.1).

Method	$N = M = 20$	$N = M = 40$	$N = M = 80$	$N = M = 160$
One-modified Crank-Nicholson	0.0137	0.0038	0.0010	0.00025
Two-modified Crank-Nicholson	0.0226	0.0071	0.0019	0.00048
Three-modified Crank-Nicholson	0.0272	0.0099	0.0028	0.00072

In the above matrices entries are given as

$$\begin{aligned}
 a_n &= -\frac{1}{2h} - \frac{nh+1}{h^2}, & b_n &= -\frac{i}{\tau}, & c_n &= \frac{i}{\tau} + \frac{2(nh+1)}{h^2}, & d_n &= \left(\frac{1}{2h} - \frac{nh+1}{h^2} \right) \\
 e_n &= -\frac{1}{4h} - \frac{nh+1}{2h^2}, & v_n &= \left(-\frac{i}{\tau} + \frac{nh+1}{h^2} \right), & s_n &= \frac{i}{\tau} + \frac{nh+1}{h^2}, & g_n &= \frac{1}{4h} - \frac{nh+1}{2h^2}.
 \end{aligned} \tag{5.7}$$

Thus, we have the second-order difference equation (5.5) with respect to n with matrix coefficients. To solve this difference equation we have applied the same modified Gauss elimination method for the difference equation with respect to n with matrix coefficients. Hence, we seek a solution of the matrix in the following form:

$$U_n = \alpha_{n+1}U_{n+1} + \beta_{n+1}, \quad n = M-1, \dots, 2, 1, 0, \tag{5.8}$$

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

$$\alpha_{n+1} = -(B_n + C_n \alpha_n)^{-1} A_n, \quad \beta_{n+1} = (B_n + C_n \alpha_n)^{-1} (D \varphi_n - C_n \beta_n), \quad n = 1, 2, 3, \dots, M-1. \tag{5.9}$$

Note that for obtaining $\alpha_{n+1}, \beta_{n+1}, n = 1, \dots, M-1$, first we need to find α_1, β_1 . As in [8], we take α_1 is an identity matrix, β_1 is the zero column vector.

For their comparison, first the errors computed by

$$E_M^N = \max_{1 \leq k \leq N-1} \left(\sum_{n=1}^{M-1} |u(t_k, x_n) - u_n^k|^2 h \right)^{1/2} \tag{5.10}$$

of the numerical solutions of problem (5.1) are recorded for different values of N and M , where $u(t_k, x_n)$ represents the exact solution and u_n^k represents the numerical solution at (t_k, x_n) . The results are shown in Table 1 for $N = M = 20, 40, 80$, and 160, respectively.

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

$$\text{rel } E_N^M = \max_{1 \leq k \leq N} \frac{E_N^M}{\left(\sum_{n=1}^M |u(t_k, x_n)|^2 h \right)^{1/2}}, \tag{5.11}$$

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

Table 2: Relative errors for the approximate solution of problem (5.1).

Method	$N = M = 20$	$N = M = 40$	$N = M = 80$	$N = M = 160$
One-modified Crank-Nicholson	0.0194	0.0054	0.0014	0.00035
Two-modified Crank-Nicholson	0.0320	0.0101	0.0027	0.00069
Three-modified Crank-Nicholson	0.0385	0.0141	0.0040	0.00100

In the article [12] it can also be found, an example that Crank-Nicolson difference scheme is divergent but modified Crank-Nicolson is convergent.

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