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A Second Order of Accuracy Difference Scheme for Schrödinger Equations with an Unknown Parameter

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Abstract. In the present study, the second order of accuracy difference scheme for numerical solution of the boundary value problem for the differential equation with an unknown parameter p

$$\begin{cases} i\frac{du(t)}{dt} + Au(t) + iu(t) = f(t) + p, \ 0 < t < T, \\ u(0) = \varphi, \ u(T) = \psi \end{cases}$$

in a Hilbert space H with self-adjoint positive definite operator A is presented. Theorem on the stability of this difference scheme is established. The stability estimates for the solution of difference schemes for two determination of an unknown parameter problem for Schrödinger equations are given.

1. Introduction. Difference scheme

The differential equations with an unknown parameter play a very important role in many branches of applied sciences and engineering (see, [1]-[3] and the references therein).

Theory and methods of solutions of differential equations with an unknown parameter have been studied extensively (see, [4]-[20] and the references therein). Note that in general such problems were not well-investigated.

In the paper [22] the boundary value problem for the Schrödinger equation with an unknown parameter p

$$\begin{cases} i\frac{du(t)}{dt} + Au(t) + iu(t) = f(t) + p, \ 0 < t < T, \\ u(0) = \varphi, \ u(T) = \psi \end{cases} \tag{1}$$

in a Hilbert space H with self-adjoint positive definite operator A was investigated. The well-posedness of this problem was established. The stability estimates for the solution of two determination of an unknown parameter problems for Schrödinger equations were obtained.

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In the paper [23], the first order of accuracy difference scheme for numerical solution of the boundary value problem (1) was presented. Theorem on the stability of this difference scheme was proved. The stability estimates for the solution of difference schemes for two determination of an unknown parameter problem for Schrödinger equations were given. It is well-known that (see [15]) modern computers allow the implementation of highly accurate ones; hence, their construction and investigation for various boundary value problems for Schrödinger equations is generating much current interest.

In the present paper the second order of accuracy Rothe difference scheme

$$\begin{cases} i\tau^{-1}(u_k - u_{k-1}) + A\left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)u_k + i\left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)u_k \\ = \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)(\varphi_k + p), \varphi_k = f\left(t_{k-\frac{1}{2}}\right), \\ t_k = k\tau,\ 1 \le k \le N,\ N\tau = T, \\ u_0 = \varphi, u_N = \psi \end{cases} \tag{2}$$

for the approximate solution of the boundary value problem (1) for the differential equation with an unknown parameter p is presented. It is clear that

$$u_k = v_k + (A + iI)^{-1} p, \tag{3}$$

$$p = (A + iI)(\psi - v_N), \tag{4}$$

where $\{v_k\}_{k=0}^N$ is the solution of the following nonlocal boundary value difference problem

$$\begin{cases} i\tau^{-1}(v_k - v_{k-1}) + A\left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)v_k + i\left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)v_k \\ = \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)\varphi_k, 1 \le k \le N, \\ v_0 - v_N = \varphi - \psi, \end{cases} \tag{5}$$

The well-posedness of difference problem (2) is established. In applications, the stability estimates for the solution of difference schemes for the approximate solution of two determination of an unknown parameter problems are obtained.

The paper is organized as follows. The section 1 is introduction. In section 2, the main theorem on stability of difference problem (2) is proved. In section 3, theorems on the stability estimates for the solution of difference schemes for the approximate solution of two determination of an unknown parameter problem are obtained. In section 4, numerical results are given. Finally, section 5 is conclusion.

2. The Main Theorem on Stability

The aim of this section, is the study of the well-posedness of the second order of accuracy difference scheme (2).

The following estimate holds:

$$\|D\|_{H\to H} \le 1,$$

Here

$$D = \left[I - i\tau(A + iI)\left[(1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right]\right]^{-1}$$

is the step operator of problem (2) for approximately solving problem (1). We state the following lemma which is needed in the sequel.

Lemma 2.1. Let A be self-adjoint positive definite operator $A \geq \delta I$.Then the operator $I - D^N$ has an inverse $T'_\tau = \left(I - D^N\right)^{-1}$and the following estimate is satisfied:

$$\| T'_\tau \|_{H\to H} \leq M(\delta). \tag{6}$$

Proof. The proof of estimate (6) is based on the triangle inequality and the estimate

$$\| \left(I - D^N\right)^{-1} \|_{H\to H} \leq \sup_{\delta\leq\mu} \frac{1}{1 - \left|1 - i\tau(\mu + i)\left(1 + \frac{\tau}{2} - i\frac{\tau\mu}{2}\right)\right|^{-N}} \leq \frac{1}{1 - (1 + \tau\delta)^{-N}} \leq M(\delta).$$

Now, let us obtain the formula for the solution of problem (2). It is clear that the second order of accuracy difference scheme

$$\begin{cases} i\tau^{-1}(u_k - u_{k-1}) + A\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)u_k + i\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)u_k \\ = \left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)(\varphi_k + p), 1 \leq k \leq N, \\ u_0 = \varphi \end{cases} \tag{7}$$

has a solution and the following formula holds:

$$u_k = D^k\varphi + \sum_{j=1}^{k}\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)D^{k-j+1}\left(p + \varphi_j\right)\tau,\ 1 \leq k \leq N. \tag{8}$$

Using condition $u_N = \psi$, we can write

$$\psi = D^N\varphi + \sum_{j=1}^{N}\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)D^{N-j+1}\varphi_j\tau$$

Since

$$\sum_{j=1}^{N}\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)D^{N-j+1}\tau = i(A + iI)^{-1}(I - D)\sum_{j=1}^{N}D^{N-j}$$

$$= i(A + iI)^{-1}(I - D^N), \tag{9}$$

we have that

$$\psi = D^N\varphi + \sum_{j=1}^{N}\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)D^{N-j+1}\varphi_j\tau + i(A + iI)^{-1}(I - D^N)p.$$

By Lemma 2.1, we get

$$p = T'_\tau\left([-i(A + iI)]\psi - D^N[-i(A + iI)]\varphi\right.$$

$$\left.-\sum_{j=1}^{N}[-i(A + iI)]\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)D^{N-j+1}\varphi_j\tau\right). \tag{10}$$

Using (8) and (10), we get

$$u_k = D^k\varphi + \sum_{j=1}^{k}\left((1 + \frac{\tau}{2})I - i\frac{\tau A}{2}\right)D^{k-j+1}\varphi_j\tau$$

$$+\sum_{j=1}^{k}\left((1+\frac{\tau}{2})I-i\frac{\tau A}{2}\right)D^{k-j+1}\tau T'_{\tau}$$
$$\times\Big([-i(A+iI)]\psi-D^{N}[-i(A+iI)]\varphi$$
$$-\sum_{j=1}^{N}[-i(A+iI)]\left((1+\frac{\tau}{2})I-i\frac{\tau A}{2}\right)D^{N-j+1}\varphi_{j}\tau\Bigg),$$
$$1\le k\le N.$$

Since

$$\sum_{j=1}^{k}\left((1+\frac{\tau}{2})I-i\frac{\tau A}{2}\right)D^{k-j+1}\tau=i(A+iI)^{-1}(I-D)\sum_{j=1}^{k}D^{k-j}$$
$$=i(A+iI)^{-1}(I-D^{k}),$$

we have that

$$u_k=R^k\varphi+\sum_{j=1}^{k}R^{k-j+1}\varphi_j\tau$$

$$u_k=D^k\varphi+\sum_{j=1}^{k}\left((1+\frac{\tau}{2})I-i\frac{\tau A}{2}\right)D^{k-j+1}\varphi_j\tau \tag{11}$$
$$+(I-D^k)T'_{\tau}\left(\psi-D^N\varphi-\sum_{j=1}^{N}\left((1+\frac{\tau}{2})I-i\frac{\tau A}{2}\right)D^{N-j+1}\varphi_j\tau\right),$$
$$1\le k\le N.$$

Hence, difference equation (2) is uniquely solvable and for the solution we have formulas (10) and (11).

Theorem 2.1. Suppose that assumptions of Lemma 2.1 hold. Then, for the solution $(\{u_k\}_{k=1}^{N}, p)$ of problem (2) in $C_\tau(H)\times H$ the estimates

$$\| p \|_H\le M\left[\|\varphi\|_H+\|\psi\|_H+\|A\varphi\|_H+\|A\psi\|_H+\|\{\varphi_k\}_{k=1}^{N}\|_{C_\tau^{(1)}(H)}\right], \tag{12}$$

$$\|\{u_k\}_{k=1}^{N}\|_{C_\tau(H)}\le M\left[\|\varphi\|_H+\|\psi\|_H+\|\{\varphi_k\}_{k=1}^{N}\|_{C_\tau(H)}\right] \tag{13}$$

hold, where M is independent of τ,φ,ψ, and $\{\varphi_k\}_{k=1}^{N}$.

Here, $C_\tau^{(1)}(H)$ is the grid space of abstract grid functions $\{f_k\}_1^N$ defined on $[0,1]_\tau$ with norm

$$\|\{f_k\}_1^N\|_{C_\tau^{(1)}(H)}=\|\{f_k\}_1^N\|_{C_\tau(H)}+\sup_{1\le k<k+r\le N}\frac{\|f_{k+r}-f_k\|_H}{r\tau},$$
$$\|\{f_k\}_1^N\|_{C_\tau(H)}=\max_{1\le k\le N}\|f_k\|_H.$$

Proof. From formulas (8) and (10) it follows that

$$p=T'_{\tau}\left[[-i(A+iI)]\psi-D^N[-i(A+iI)]\varphi-\varphi_N+D^N\varphi_1-\sum_{j=2}^{N}D^{N-j+1}\left(\varphi_{j-1}-\varphi_j\right)\right].$$

Using this formula, the triangle inequality and estimate (6), we obtain

$$\| p \|_H \leq \| T'_\tau \|_{H\to H} \Big(\left\|[-i(A+iI)]\psi\right\|_H + \left\|D^N\right\|_{H\to H} \left\|[-i(A+iI)]\varphi\right\|_H$$

$$+ \sum_{j=2}^{N} \left\|D^{N-j+1}\right\|_{H\to H} \left\|\varphi_j - \varphi_{j-1}\right\|_H + \left\|\varphi_N\right\| + \left\|D^N\right\|_{H\to H} \left\|\varphi_1\right\|_H \Big)$$

$$\leq M\left[\| \varphi \|_H + \| \psi \|_H + \| A\varphi \|_H + \| A\psi \|_H + \| \{A\varphi_k\}_{k=1}^N \|_{C_\tau^{(1)}(H)}\right].$$

Estimate (12) is proved. Using formula (11), the triangle inequality and estimate (6), we obtain

$$\| u_k \|_H \leq \Bigg(\left\| \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right) D^k \right\|_{H\to H} \left\|\varphi\right\|_H$$

$$+ \sum_{j=1}^{k} \left\| \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right) D^{k-j+1} \right\|_{H\to H} \left\|\varphi_j\right\|_H \tau + \left(1 + \left\|D^k\right\|_{H\to H}\right) \| T'_\tau \|_{H\to H}$$

$$\times \left(\| \psi \|_H + \left\|D^N\right\|_{H\to H} \left\|\varphi\right\|_H + \sum_{j=1}^{N} \left\| \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right) D^{k-j+1} \right\|_{H\to H} \left\|\varphi_j\right\|_H \tau \right) \Bigg)$$

$$\leq M\left[\| \varphi \|_H + \| \psi \|_H + \| \{\varphi_k\}_{k=1}^N \|_{C_\tau(H)}\right]$$

for any k. From that it follows estimate (13). Theorem 2.1 is proved.

3. Applications

In this section, we consider the applications of main Theorem 2.1.

First, the nonlocal boundary value problem for the Schrödinger equation

$$\begin{cases} iu_t - (a(x)u_x)_x + \delta u + iu = p(x) + f(t,x),\ 0 < t < T,\ 0 < x < 1, \\ u(0,x) = \varphi(x), u(T,x) = \psi(x), 0 \leq x \leq 1, \\ u(t,0) = u(t,1),\ u_x(t,0) = u_x(t,1),\ 0 \leq t \leq T \end{cases} \tag{14}$$

is considered. Problem (14) has a unique smooth solution $(u(t,x), p(x))$ for the smooth functions $a(x) \geq a > 0$, $x \in (0,1)$, $\delta > 0$, $a(1) = a(0)$, $\varphi(x)$, $\psi(x)$ $(x \in [0,1])$ and $f(t,x)$ $(t \in (0,T), x \in (0,1))$. This allows us to reduce the nonlocal boundary values problem (14) to the nonlocal boundary value problem (1) in a Hilbert space $H = L_2[0,1]$ with a self-adjoint positive definite operator A^x defined by formula

$$A^x u(x) = -(a(x)u_x)_x + \delta u \tag{15}$$

with domain

$$D(A^x) = \{u(x) : u(x), u_x(x), (a(x)u_x)_x \in L_2[0,1], u(1) = u(0), u_x(1) = u_x(0)\}.$$

The discretization of problem (14) is carried out in two steps. In the first step, we define the grid space

$$[0,1]_h = \{x = x_n : x_n = nh,\ 0 \leq n \leq M,\ Mh = 1\}.$$

Let us introduce the Hilbert space $L_{2h} = L_2([0,1]_h)$ of the grid functions $\varphi^h(x) = \{\varphi_n\}_1^{M-1}$ defined on $[0,1]_h$, equipped with the norm

$$\|\varphi^h\|_{L_{2h}} = \left(\sum_{x\in[0,1]_h} |\varphi(x)|^2 h \right)^{1/2}.$$

To the differential operator A^x defined by formula (15), we assign the difference operator A_h^x by the formula

$$A_h^x \varphi^h(x) = \{-(a(x)\varphi_{\bar{x}})_{x,n} + \delta\varphi_n\}_1^{M-1} \tag{16}$$

acting in the space of grid functions $\varphi^h(x) = \{\varphi_n\}_1^{M-1}$ satisfying the conditions $\varphi_0 = \varphi_M$, $\varphi_1 - \varphi_0 = \varphi_M - \varphi_{M-1}$. It is well-known that A_h^x is a self-adjoint positive definite operator in L_{2h}. With the help of A_h^x, we reach the boundary value problem

$$\begin{cases} i\frac{du^h(t,x)}{dt} + A_h^x u^h(t,x) + iu^h(t,x) = p^h(x) + f^h(t,x),\ 0 < t < T,\ x \in [0,1]_h, \\ u^h(0,x) = \varphi^h(x), u^h(T,x) = \psi^h(x), x \in [0,1]_h. \end{cases} \tag{17}$$

In the second step, we replace (17) with the difference scheme (2)

$$\begin{cases} i\frac{u_k^h(x)-u_{k-1}^h(x)}{\tau} + A_h^x\left((1+\frac{\tau}{2})I - i\frac{\tau A_h^x}{2}\right)u_k^h(x) + i\left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)u_k^h(x) \\ = \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)\left(p^h(x) + f_k^h(x)\right), \\ f_k^h(x) = f^h(t_k - \frac{\tau}{2}, x),\ t_k = k\tau,\ 1 \le k \le N,\ x \in [0,1]_h, \\ u^h(0,x) = \varphi^h(x),\ u^h(1,x) = \psi^h(x),\ x \in [0,1]_h. \end{cases} \tag{18}$$

Theorem 3.1. The solution pairs $\left(\left\{u_k^h(x)\right\}_0^N, p^h(x)\right)$ of problem (18) satisfy the stability estimates

$$\| p^h \|_{L_{2h}} \le M_1 \left[\|\varphi^h\|_{L_{2h}} + \|\psi^h\|_{L_{2h}} + \|A_h^x\varphi^h\|_{L_{2h}} + \|A_h^x\psi^h\|_{L_{2h}} + \| \left\{f_k^h\right\}_1^N \|_{C_\tau^{(1)}(L_{2h})} \right],$$

$$\| \left\{u_k^h\right\}_1^N \|_{C_\tau(L_{2h})} \le M_2 \left[\|\varphi^h\|_{L_{2h}} + \|\psi^h\|_{L_{2h}} + \| \left\{f_k^h\right\}_1^N \|_{C_\tau(L_{2h})} \right],$$

where M_1 and M_2 does not depend on $\tau, h, \varphi^h, \psi^h$ and $f_k^h, 1 \le k \le N$. Here $C_\tau^{(1)}(L_{2h})$ is the grid space of grid functions $\left\{f_k^h\right\}_1^N$ defined on $[0,1]_\tau \times [0,1]_h$ with norm

$$\| \left\{f_k^h\right\}_1^N \|_{C_\tau^{(1)}(L_{2h})} = \| \left\{f_k^h\right\}_1^N \|_{C_\tau(L_{2h})} + \sup_{1\le k<k+r\le N} \frac{\|f_{k+r}^h - f_k^h\|_{L_{2h}}}{r\tau},$$

$$\| \left\{f_k^h\right\}_1^N \|_{C_\tau(L_{2h})} = \max_{1\le k\le N} \|f_k^h\|_{L_{2h}}.$$

The proof of Theorem 3.1 is based on the abstract Theorem 2.1 and the symmetry property of the difference operator A_h^x.

Second, let $\Omega = (x = (x_1, \cdots, x_n) : 0 < x_k < 1, k = 1, \cdots, n)$ be the unit open cube in the n-dimensional Euclidean space $\mathbb{R}^n$ with boundary S, $\overline{\Omega} = \Omega \cup S$. In $[0, T] \times \Omega$, the boundary value problem for the multi-dimensional Schrödinger equation

$$\begin{cases} i\frac{\partial u(t,x)}{\partial t} - \sum\limits_{r=1}^{n} (a_r(x)u_{x_r})_{x_r} + iu = p(x) + f(t, x), \\ x = (x_1, \ldots, x_n) \in \Omega, \ 0 < t < T, \\ u(0, x) = \varphi(x), u(T, x) = \psi(x), x \in \overline{\Omega}, \\ u(t, x) = 0, \ x \in S, \ 0 \leq t \leq T \end{cases} \tag{19}$$

is considered. Here $a_r(x) \geq a > 0$, $(x \in \Omega)$, $\varphi(x)$, $\psi(x)$ $(x \in \overline{\Omega})$, and $f(t, x)$ $(t \in (0, T), \ x \in \Omega)$ are given smooth functions.

We consider the Hilbert space $L_2(\overline{\Omega})$ of the all square integrable functions defined on $\overline{\Omega}$, equipped with the norm

$$\| f \|_{L_2(\overline{\Omega})} = \left(\int \cdots \int_{x \in \overline{\Omega}} |f(x)|^2 dx_1 \cdots dx_n \right)^{\frac{1}{2}}.$$

Problem (19) has a unique smooth solution $(u(t, x), p(x))$ for the smooth functions $\varphi(x)$, $\psi(x)$, $a_r(x)$ and $f(t, x)$. This allows us to reduce the problem (19) to the nonlocal boundary value problem (1) in the Hilbert space $H = L_2(\overline{\Omega})$ with a self-adjoint positive definite operator A^x defined by formula

$$A^x u(x) = -\sum_{r=1}^{n} (a_r(x)u_{x_r})_{x_r} \tag{20}$$

with domain

$$D(A^x) = \left\{ u(x) : u(x), u_{x_r}(x), (a_r(x)u_{x_r})_{x_r} \in L_2(\overline{\Omega}), 1 \leq r \leq n, u(x) = 0, x \in S \right\}.$$

The discretization of problem (19) is carried out in two steps. In the first step, we define the grid space

$$\overline{\Omega}_h = \{x = x_r = (h_1 j_1, \cdots, h_n j_n), j = (j_1, \cdots, j_n), 0 \leq j_r \leq N_r,$$
$$N_r h_r = 1, r = 1, \cdots, n\}, \Omega_h = \overline{\Omega}_h \cap \Omega, S_h = \overline{\Omega}_h \cap S$$

and introduce the Hilbert space $L_{2h} = L_2(\overline{\Omega}_h)$ of the grid functions

$$\varphi^h(x) = \{\varphi(h_1 j_1, \cdots, h_n j_n)\}$$

defined on $\overline{\Omega}_h$ equipped with the norm

$$\left\|\varphi^h\right\|_{L_{2h}} = \left(\sum_{x \in \Omega_h} \left|\varphi^h(x)\right|^2 h_1 \cdots h_n \right)^{\frac{1}{2}}.$$

To the differential operator A^x defined by formula (20), we assign the difference operator A_h^x by the formula

$$A_h^x u^h = -\sum_{r=1}^{n} \left(\alpha_r(x) u_{x_r}^h\right)_{x_r, j_r},$$

where A_h^x is known as self-adjoint positive definite operator in L_{2h}, acting in the space of grid functions $u^h(x)$ satisfying the conditions $u^h(x) = 0$ for all $x \in S_h$. With the help of the difference operator A_h^x, we arrive the following boundary value problem

$$\begin{cases} iu_t^h(t,x) + A_h^x u^h(t,x) + iu^h(t,x) = p^h(x) + f^h(t,x), \\ 0 < t < T, x \in \Omega_h, \\ u^h(0,x) = \varphi^h(x),\ u^h(T,x) = \psi^h(x), x \in \Omega_h \end{cases} \tag{21}$$

for an infinite system of ordinary differential equations. In the second step, we replace (21) with the difference scheme (2)

$$\begin{cases} i\frac{u_k^h(x)-u_{k-1}^h(x)}{\tau} + A_h^x\left((1+\frac{\tau}{2})I - i\frac{\tau A_h^x}{2}\right)u_k^h(x) + i\left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)u_k^h(x) \\ = \left((1+\frac{\tau}{2})I - i\frac{\tau A}{2}\right)\left(p^h(x) + f_k^h(x)\right), \\ f_k^h(x) = f^h(t_k - \frac{\tau}{2}, x),\ t_k = k\tau,\ 1 \le k \le N,\ x \in \Omega_h, \\ u^h(0,x) = \varphi^h(x),\ u^h(1,x) = \psi^h(x),\ x \in \Omega_h. \end{cases} \tag{22}$$

Theorem 3.2. The solution pairs $\left(\left\{u_k^h(x)\right\}_0^N, p^h(x)\right)$ of problem (22) satisfy the stability estimates

$$\| p^h \|_{L_{2h}} \le M_1 \left[\|\varphi^h\|_{L_{2h}} + \|\psi^h\|_{L_{2h}} + \|A_h^x\psi^h\|_{L_{2h}} + \| \left\{f_k^h\right\}_1^N \|_{C_\tau^{(1)}(L_{2h})}\right],$$

$$\| \left\{u_k^h\right\}_1^N \|_{C_\tau(L_{2h})} \le M_2 \left[\|\varphi^h\|_{L_{2h}} + \|\psi^h\|_{L_{2h}} + \| \left\{f_k^h\right\}_1^N \|_{C_\tau(L_{2h})}\right],$$

where M_1 and M_2 is independent of $\tau, h, \varphi^h, \psi^h$ and $f_k^h, 1 \le k \le N$. Here $C_\tau^{(1)}(L_{2h})$ is the grid space of grid functions $\left\{f_k^h\right\}_1^N$ defined on $[0,1]_\tau \times \overline{\Omega_h}$ with norm

$$\| \left\{f_k^h\right\}_1^N \|_{C_\tau^{(1)}(L_{2h})} = \| \left\{f_k^h\right\}_1^N \|_{C_\tau(L_{2h})} + \sup_{1\le k<k+r\le N} \frac{\|f_{k+r}^h - f_k^h\|_{L_{2h}}}{r\tau},$$

$$\| \left\{f_k^h\right\}_1^N \|_{C_\tau(L_{2h})} = \max_{1\le k\le N} \|f_k^h\|_{L_{2h}}.$$

The proof of Theorem 3.2 is based on Theorem 2.1 and the symmetry property of the difference operator A_h^x defined by formula (19) and the following theorem on the coercivity inequality for the solution of the elliptic difference problem in L_{2h}.

Theorem 3.3. For the solutions of the elliptic difference problem [21]

$$\begin{cases} A_h^x u^h(x) = \omega^h(x),\ x \in \Omega_h, \\ u^h(x) = 0,\ x \in S_h, \end{cases} \tag{23}$$

the following coercivity inequality holds:

$$\sum_{r=1}^n \left\|u^h{}_{x_r x_{\bar r}}\right\|_{L_{2h}} \le M\|\omega^h\|_{L_{2h}},$$

where M does not depend on h and ω^h.

4. A Numerical Result

In present section, the numerical analysis of approximate solution of the boundary value problem

$$\begin{cases} i\frac{\partial u(t,x)}{\partial t} - \frac{\partial^2 u(t,x)}{\partial x^2} + iu(t,x) = p(x) + f(t,x), x \in (0,\pi), \ t \in (0,1), \\ u(0,x) = \sin x, \ u(1,x) = e^{-1}\sin x, \ x \in [0,\pi], \\ u(t,0) = u(t,\pi) = 0, \ t \in [0,1] \end{cases} \tag{24}$$

is given. It is clear that the exact solution of problem (24) is $u(t,x) = e^{-t}\sin x$ and $p(x) = \sin x$. Using (2) for the approximate solution of (24), we get the following second order of accuracy difference scheme

$$\begin{cases} i\dfrac{u_n^k - u_n^{k-1}}{\tau} - (1+\frac{\tau}{2})\dfrac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{h^2} \\ -i\dfrac{\tau}{2}\left(\dfrac{u_{n+2}^k - 4u_{n+1}^k + 6u_n^k - 4u_{n-1}^k + u_{n-2}^k}{h^4}\right) \\ +i(1+\frac{\tau}{2})u_n^k - \frac{\tau}{2}\dfrac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{h^2} \\ = \theta_n^k, \ \theta_n^k = (1+\frac{\tau}{2})f(t_k - \frac{\tau}{2}, x_n) \\ +i\dfrac{\tau}{2}\left(\dfrac{f(t_k - \frac{\tau}{2}, x_{n+1}) - 2f(t_k - \frac{\tau}{2}, x_n) + f(t_k - \frac{\tau}{2}, x_{n-1})}{h^2}\right) \\ +(1+\frac{\tau}{2})p(x_n) + i\dfrac{\tau}{2}\left(\dfrac{p(x_{n+1}) - 2p(x_n) + p(x_{n-1})}{h^2}\right), \\ t_k = k\tau, \ 1 \le k \le N, \\ N\tau = T, \ x_n = nh, 2 \le n \le M-2, Mh = \pi, \\ u_n^0 = \sin(x_n), u_n^N = e^{-1}\sin(x_n), x_n = nh, 0 \le n \le M, \\ u_0^k = u_M^k = 0, 0 \le k \le N, \\ 2u_0^k - 5u_1^k + 4u_2^k - u_3^k = u_{M-3}^k - 4u_{M-2}^k + 5u_{M-1}^k - 2u_M^k = 0, 0 \le k \le N. \end{cases} \tag{25}$$

For obtaining the values of $p(x_n)$ at the grid points we will use formula

$$p(x_n) = -e^{-1}\frac{\sin(x_{n+1}) - 2\sin(x_n) + \sin(x_{n-1})}{h^2} + ie^{-1}\sin(x_n)$$

$$+\frac{v_{n+1}^N - 2v_n^N + v_{n-1}^N}{h^2} - iv_n^N, x_n = nh, 1 \le n \le M-1, \tag{26}$$

where $v_s^k, s = n \pm 1, n$ is the solution of the second order of accuracy difference scheme

$$\begin{cases} i\dfrac{v_n^k - v_n^{k-1}}{\tau} - (1+\frac{\tau}{2})\dfrac{v_{n+1}^k - 2v_n^k + v_{n-1}^k}{h^2} \\ -i\dfrac{\tau}{2}\left(\dfrac{v_{n+2}^k - 4v_{n+1}^k + 6v_n^k - 4v_{n-1}^k + v_{n-2}^k}{h^4}\right) + i(1+\frac{\tau}{2})v_n^k \\ -\frac{\tau}{2}\dfrac{v_{n+1}^k - 2v_n^k + v_{n-1}^k}{h^2} = \phi_n^k,\ \phi_h^k = (1+\frac{\tau}{2})f(t_k - \frac{\tau}{2}, x_n) \\ +i\dfrac{\tau}{2}\left(\dfrac{f(t_k - \frac{\tau}{2}, x_{n+1}) - 2f(t_k - \frac{\tau}{2}, x_n) + f(t_k - \frac{\tau}{2}, x_{n-1})}{h^2}\right), \\ t_k = k\tau,\ 1 \le k \le N,\ N\tau = T,\ \ x_n = nh, 2 \le n \le M-2\ , Mh = \pi, \\ v_n^N - v_n^0 = \left(e^{-1} - 1\right)\sin(x_n)\,, x_n = nh, 0 \le n \le M, \\ v_0^k = v_M^k = 0, 0 \le k \le N, \\ 2v_0^k - 5v_1^k + 4v_2^k - v_3^k = v_{M-3}^k - 4v_{M-2}^k + 5v_{M-1}^k - 2v_M^k = 0, 0 \le k \le N \end{cases} \tag{27}$$

is generated by difference scheme (5).

Applying the difference scheme (27), we obtain $(N+1)\times(M+1)$ system of linear equations and we can write them in the matrix form as

$$\begin{aligned} &Av_{n+2} + Bv_{n+1} + Cv_n + Dv_{n-1} + Ev_{n-2} = I\phi_n, \quad 2 \le n \le M-2, \\ &v_0 = v_M = \widetilde{0}, v_1 = \frac{4}{5}v_2 - \frac{1}{5}v_3, v_{M-1} = \frac{4}{5}v_{M-2} - \frac{1}{5}v_{M-3}, \end{aligned} \tag{28}$$

where

$$E = A = \begin{bmatrix} 0 & 0 & 0 & . & 0 & 0 & 0 & 0 \\ 0 & \alpha & 0 & . & 0 & 0 & 0 & 0 \\ 0 & 0 & \alpha & . & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 0 & 0 & \alpha & 0 \\ 0 & 0 & 0 & . & 0 & 0 & 0 & \alpha \end{bmatrix}_{(N+1)\times(N+1)},$$

$$D = B = \begin{bmatrix} 0 & 0 & 0 & . & 0 & 0 & 0 & 0 \\ 0 & \beta & 0 & . & 0 & 0 & 0 & 0 \\ 0 & 0 & \beta & . & 0 & 0 & 0 & 0 \\ . & . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & 0 & 0 & \beta & 0 \\ 0 & 0 & 0 & . & 0 & 0 & 0 & \beta \end{bmatrix}_{(N+1)\times(N+1)},$$

and

$$C = \begin{bmatrix} -1 & 0 & 0 & . & 0 & 0 & 1 \\ \sigma & \gamma & 0 & . & 0 & 0 & 0 \\ 0 & \sigma & \gamma & . & 0 & 0 & 0 \\ . & . & . & . & . & . & . \\ 0 & 0 & 0 & . & \sigma & \gamma & 0 \\ 0 & 0 & 0 & . & 0 & \sigma & \gamma \end{bmatrix}_{(N+1)\times(N+1)}, I = \begin{bmatrix} 1 & 0 & . & 0 \\ 0 & 1 & . & 0 \\ . & . & . & . \\ 0 & 0 & . & 1 \end{bmatrix}_{(N+1)\times(N+1)}.$$

Here,

$$\alpha=-i\frac{\tau}{2h^4},\beta=-\frac{1}{h^2}-\frac{\tau}{h^2}+i\frac{2\tau}{h^4},\gamma=i\frac{1}{\tau}+\frac{2}{h^2}-i\frac{3\tau}{h^4}+\frac{2\tau}{h^2}+i+i\frac{\tau}{2},\sigma=-\frac{i}{\tau}.$$

By using modified Gauss elimination method, we can reach the solution of $v_n^k, 0\le k\le N,\ 0\le n\le M$. For the solution of the matrix equations, we seek formula for the solution of the form

$$\begin{cases} v_n=\alpha_{n+1}v_{n+1}+\beta_{n+1}v_{n+2}+\gamma_{n+1},\ n=M-2,\cdots,2,1,\\ v_M=\widetilde{0},\\ v_{M-1}=\left[(\beta_{M-2}+5I)-(4I-\alpha_{M-2})\,\alpha_{M-1}\right]^{-1}\left[(4I-\alpha_{M-2})\,\gamma_{M-1}-\gamma_{M-2}\right], \end{cases}$$

where α_j,β_j and $\gamma_j,\ j=1,\cdots M-1$ are calculated as

$$\begin{aligned} \alpha_{n+1}&=-\left(C+D\alpha_n+E\beta_{n-1}+E\alpha_{n-1}\alpha_n\right)^{-1}\left(B+D\varphi_n+E\alpha_{n-1}\beta_n\right),\\ \beta_{n+1}&=-\left(C+D\alpha_n+E\beta_{n-1}+E\alpha_{n-1}\alpha_n\right)^{-1}(A),\\ \gamma_{n+1}&=\left(C+D\alpha_n+E\beta_{n-1}+E\alpha_{n-1}\alpha_n\right)^{-1}\left(I\varphi_n-D\gamma_n-E\alpha_{n-1}\gamma_n-E\gamma_{n-1}\right) \end{aligned}$$

with α_1 and β_1 are $(N+1)\times(N+1)$ and γ_1 and γ_2 are $(N+1)\times 1$ zero matrices and

$$\alpha_2=\begin{bmatrix} \frac{4}{5} & 0 & . & 0\\ 0 & \frac{4}{5} & . & 0\\ . & . & . & .\\ 0 & 0 & . & \frac{4}{5} \end{bmatrix}_{(N+1)\times(N+1)},\ \beta_2=\begin{bmatrix} -\frac{1}{5} & 0 & . & 0\\ 0 & -\frac{1}{5} & . & 0\\ . & . & . & .\\ 0 & 0 & . & -\frac{1}{5} \end{bmatrix}_{(N+1)\times(N+1)}.$$

Then, applying the second order of accuracy difference scheme (25), we have again $(N+1)\times(N+1)$ system of linear equations and we write them in the matrix form as

$$\begin{aligned} &A_2u_{n+2}+B_2u_{n+1}+C_2u_n+D_2u_{n-1}+E_2u_{n-2}=I\theta_n,\quad 2\le n\le M-2,\\ &u_0=u_M=\widetilde{0},u_1=\frac{4}{5}u_2-\frac{1}{5}u_3,u_{M-1}=\frac{4}{5}u_{M-2}-\frac{1}{5}u_{M-3}, \end{aligned} \tag{29}$$

$$A_2=A,\ B_2=B,D_2=D,E_2=E,$$

and

$$C_2=\begin{bmatrix} 1 & 0 & 0 & . & 0 & 0 & 0\\ \sigma & \gamma & 0 & . & 0 & 0 & 0\\ 0 & \sigma & \gamma & . & 0 & 0 & 0\\ . & . & . & . & . & . & .\\ 0 & 0 & 0 & . & \sigma & \gamma & 0\\ 0 & 0 & 0 & . & 0 & \sigma & \gamma \end{bmatrix}_{(N+1)\times(N+1)},$$

where

$$\gamma=i\frac{1}{\tau}+\frac{2}{h^2}-i\frac{3\tau}{h^4}+\frac{2\tau}{h^2}+i+i\frac{\tau}{2},\sigma=-\frac{i}{\tau}.$$

Applying modified Gauss elimination method, we can reach the solution of $u_n^k, 0\le k\le N,\ 0\le n\le M$. We will give the results of the numerical analysis. The numerical solutions are recorded for different values of N and M and u_n^k represents the numerical solutions of these difference scheme at (t_k,x_n). Table 1 is constructed for $N=M=20, 40$ and 80 respectively and the error is computed by the following formula.

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

Table 1. Error analysis for the exact solution $u(t,x)$.

Method	N=M=20	N=M=40	N=M=80
1st order of accuracy d.s.	0.0024	0.0012	6.0463×10^{-4}
2nd order of accuracy d.s.	3.0543×10^{-4}	7.4075×10^{-4}	1.8351×10^{-5}

For their comparison, Table 2 is constructed when errors are computed by

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

Table 2. Error analysis for the exact solution $u(t,x)$.

Method	N=M=20	N=M=40	N=M=80
1st order of accuracy d.s.	0.0019	9.5692×10^{-4}	4.8241×10^{-4}
2nd order of accuracy d.s.	2.7818×10^{-4}	6.1783×10^{-4}	1.4793×10^{-5}

Table 3. Error analysis for $p(x)$.

	N=20	N=40	N=80
1st order of accuracy d.s.	0.0145	0.0072	0.0036
2nd order of accuracy d.s.	0.0017	4.3813×10^{-4}	1.0884×10^{-4}

Thus, by using the second order of accuracy difference scheme the solution accuracy increases faster than the first order of accuracy difference scheme. Therefore, the theoretical result for the solution of difference scheme, the second order of accuracy is supported by the result of this numerical example.

5. Conclusion

In the present paper, the well-posedness of the second order of accuracy difference scheme for the approximate solution of determination of an unknown parameter problem for the Schrödinger equation is established. In applications, the stability estimates for the solution of difference schemes of the approximate solution of two determination of an unknown parameter problem are obtained. Moreover, applying the result of the monograph [15] the high order of accuracy single-step difference schemes for the numerical solution of the boundary value problem (1) can be presented. Of course, the stability estimates for the solution of these difference schemes have been established without any assumptions about the grid steps τ in t and h in space variables.

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