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On the Crank-Nicolson difference scheme for the time-dependent source identification problem

In this study the source identification problem for the one-dimensional Schrödinger equation with non-local boundary conditions is considered. A second order of accuracy Crank-Nicolson difference scheme for the numerical solution of the differential problem is presented. Stability estimates are proved for the solution of this difference scheme. Numerical results are given.

Keywords: identification problem, Schrödinger equation, difference scheme, Crank-Nicolson, stability.

Introduction

Source identification problems (SIPs) have the significant role in natural science, applied sciences, engineering, quantum mechanics, diffusion equations, heat equations (see [1–4] and references therein). The theory and applications of SIPs for partial differential equations (PDEs) were studied in many works (see [5–32] and references therein). The time-dependent SIP

$$\begin{cases} i \frac{\partial u(t,x)}{\partial t} - \frac{\partial}{\partial x} \left(a(x) \frac{\partial u(t,x)}{\partial x} \right) + \delta u(t,x) \\ = p(t)q(x) + f(t,x), t \in (0, T), x \in (0, l), \\ u(0, x) = \varphi(x), x \in [0, l], \\ u(t, 0) = u(t, l), u_x(t, 0) = u_x(t, l), \\ \int_0^l u(t, x) dx = \zeta(t), t \in [0, T] \end{cases} \quad (1)$$

for the one-dimensional Schrödinger equation (SE) was investigated [33]. Here $0 < a \leq a(x)$, $f(t, x)$, $\zeta(t)$, $\varphi(x)$, $q(x)$ and $a(x)$ are given sufficiently smooth functions and $q(0) = q(l)$, $q'(0) = q'(l)$ and $\int_0^l q(x) dx \neq 0$. Stability estimates were established for the solution of source identification problem (1). A first order of accuracy difference scheme was investigated for the numerical solution of this problem.

In this paper a second order of accuracy Crank-Nicolson difference scheme for the numerical solution of problem (1) is presented. Stability estimates are proved for the solution of the difference scheme. Numerical results are provided.

Stability of difference problem

To formulate results on difference problem we introduce the normed space. Let $C_\tau(H) = C([0, T]_\tau, H)$ of all mesh functions $\phi^\tau = \{\phi_k\}_{k=0}^N$ defined on

$$[0, T]_\tau = \{t_k = k\tau, 0 \leq k \leq N, N\tau = T\}$$

with values in H equipped with the norm

$$\|\phi^\tau\|_{C_\tau(H)} = \max_{0 \leq k \leq N} \|\phi_k\|_H.$$

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Moreover, $L_{2h} = L_2 [0, l]_h$ are normed spaces of all mesh functions $\gamma^h(x) = \{\gamma_n\}_{n=0}^M$ defined on

$$[0, l]_h = \{x_n = nh, 0 \leq n \leq M, Mh = l\}$$

equipped with the norm

$$\|\gamma^h\|_{L_{2h}} = \left\{ \sum_{i=0}^M |\gamma_i|^2 h \right\}^{\frac{1}{2}},$$

and $W_{2h}^2 = W_2^2 [0, l]_h$ is the Sobolev space with norm

$$\|\gamma^h\|_{W_{2h}^2} = \left\{ \sum_{i=0}^M |\gamma_i|^2 h + \sum_{i=1}^{M-1} \left| \frac{\gamma_{i+1} - 2\gamma_i + \gamma_{i-1}}{h^2} \right|^2 h \right\}^{\frac{1}{2}}.$$

To the differential operator A defined by (2) we introduce the difference operator A^h defined by the formula

$$A^h \psi^h(x) = \left\{ -\frac{1}{h} \left(a_{n+1} \frac{\psi_{n+1} - \psi_n}{h} - a_n \frac{\psi_n - \psi_{n-1}}{h} \right) + \delta \psi_n \right\}_{n=1}^{M-1}, a_n = a(x_n) \quad (2)$$

acting in the space of grid functions $\psi^h(x) = \{\psi_n\}_{n=0}^M$ defined on $[0, l]_h$ satisfying the conditions $\psi_M^k = \psi_0^k$, $\psi_M^k - \psi_{M-1}^k = \psi_1^k - \psi_0^k$. For the numerical solution $\{u_n^\tau\}_{n=0}^M$ of problem (1) we consider the second order of accuracy Crank-Nicolson difference scheme

$$\begin{cases} i \frac{u_n^k - u_{n-1}^{k-1}}{\tau} - \frac{1}{2h} \left(a_{n+1} \frac{u_{n+1}^k - u_n^k}{h} - a_n \frac{u_n^k - u_{n-1}^k}{h} \right) \\ - \frac{1}{2h} \left(a_{n+1} \frac{u_{n+1}^{k-1} - u_n^{k-1}}{h} - a_n \frac{u_n^{k-1} - u_{n-1}^{k-1}}{h} \right) + \delta \frac{u_n^k + u_n^{k-1}}{2} \\ = \frac{p_k + p_{k-1}}{2} q_n + f_k(x_n), f_k(x_n) = f\left(t_k - \frac{\tau}{2}, x_n\right), \\ a_n = a(x_n), q_n = q(x_n), 1 \leq k \leq N, 1 \leq n \leq M-1, \\ u_n^0 = \varphi_n, \varphi_n = \varphi(x_n), 0 \leq n \leq M, \\ u_M^k = u_0^k, u_M^k - u_{M-1}^k = u_1^k - u_0^k, \sum_{i=1}^M u_i^k h = \zeta_k, \\ \zeta_k = \zeta(t_k), 0 \leq k \leq N. \end{cases} \quad (3)$$

Let us give the following result on the stability of DS (3).

Theorem 1. For the solution of DS (3) the stability estimates are satisfied:

$$\begin{aligned} & \left\| \left\{ \frac{1}{\tau} (u_k^h - u_{k-1}^h) \right\}_{k=1}^N \right\|_{C_\tau(L_{2h})} + \left\| \left\{ \frac{u_k^h + u_{k-1}^h}{2} \right\}_{k=1}^N \right\|_{C_\tau(W_{2h}^2)} + \left\| \left\{ \frac{p_k + p_{k-1}}{2} \right\}_{k=1}^N \right\|_{C[0, T]_\tau} \\ & \leq Q(q) \left[\|\varphi^h\|_{W_{2h}^2} + \|f_1^h\|_{L_{2h}} + |\zeta_0| \right. \\ & \left. + \left\| \left\{ \frac{1}{\tau} (f_k^h - f_{k-1}^h) \right\}_{k=2}^N \right\|_{C_\tau(L_{2h})} + \left\| \left\{ \frac{1}{\tau} (\zeta_k - \zeta_{k-1}) \right\}_{k=1}^N \right\|_{C[0, T]_\tau} \right]. \end{aligned}$$

Proof. Denote that

$$u_n^k = w_n^k - i\eta_k q_n, \quad (4)$$

where

$$\frac{p_k + p_{k-1}}{2} = \frac{\eta_k - \eta_{k-1}}{\tau}, 1 \leq k \leq N, \eta_0 = 0 \quad (5)$$

and w_n^k is the solution of the following Crank-Nicolson difference scheme

$$\left\{ \begin{aligned} & i \frac{w_n^k - w_n^{k-1}}{\tau} - \frac{1}{2h} \left(a_{n+1} \frac{w_{n+1}^k - w_n^k}{h} - a_n \frac{w_n^k - w_{n-1}^k}{h} \right) \\ & - \frac{1}{2h} \left(a_{n+1} \frac{w_{n+1}^{k-1} - w_n^{k-1}}{h} - a_n \frac{w_n^{k-1} - w_{n-1}^{k-1}}{h} \right) + \delta \frac{w_n^k + w_n^{k-1}}{2} \\ & = f_k(x_n) - i \frac{\eta_k + \eta_{k-1}}{2} \left[-\frac{1}{2h} \left(a_{n+1} \frac{q_{n+1} - q_n}{h} - a_n \frac{q_n - q_{n-1}}{h} \right) + \delta q_n \right], \\ & 1 \leq k \leq N, 1 \leq n \leq M - 1, \\ & w_n^0 = \varphi_n, 0 \leq n \leq M, \\ & w_M^k = w_0^k, u_M^k - u_{M-1}^k = u_1^k - u_0^k, 0 \leq k \leq N. \end{aligned} \right. \quad (6)$$

Now, we estimate $|\frac{p_k + p_{k-1}}{2}|$. Using the conditions $\sum_{m=1}^M u_m^k h = \zeta_k$ and (4), we obtain

$$\eta_k = \frac{i}{d_1} \left(\sum_{m=1}^M w_m^k h - \zeta_k \right), d_1 = \sum_{m=1}^M q_m h, 1 \leq k \leq N,$$

$$\frac{p_k + p_{k-1}}{2} = \frac{\sum_{m=1}^M (w_m^k - w_m^{k-1}) h - (\zeta_k - \zeta_{k-1})}{i \tau d}, 1 \leq k \leq N.$$

Using the Cauchy-Schwartz inequality and triangle inequality, we get

$$\begin{aligned} & \left| \frac{p_k + p_{k-1}}{2} \right| \\ & \leq Q_1(q) \left(\left\| \left\{ \frac{w_m^k - w_m^{k-1}}{\tau} \right\}_{m=1}^M \right\|_{L_{2h}} + \left| \frac{\zeta_k - \zeta_{k-1}}{\tau} \right| \right) \end{aligned}$$

for all $1 \leq k \leq N$ and

$$\begin{aligned} & \left\| \left\{ \frac{p_k + p_{k-1}}{2} \right\}_{k=1}^N \right\|_{C[0,T]_\tau} \\ & \leq Q_1(q) \left[\left\| \left\{ \frac{1}{\tau} (w_k^h - w_{k-1}^h) \right\}_{k=1}^N \right\|_{C_\tau(L_{2h})} + \left\| \left\{ \frac{\zeta_k - \zeta_{k-1}}{\tau} \right\}_{k=1}^N \right\|_{C[0,T]_\tau} \right]. \end{aligned}$$

Now, applying formulas (4) and (5), we obtain

$$\frac{u_n^k - u_n^{k-1}}{\tau} = \frac{w_n^k - w_n^{k-1}}{\tau} - i \frac{p_k + p_{k-1}}{2} q_n$$

and

$$\begin{aligned} & \left\| \left\{ \frac{1}{\tau} (u_k^h - u_{k-1}^h) \right\}_{k=1}^N \right\|_{C_\tau(L_{2h})} \leq \left\| \left\{ \frac{1}{\tau} (w_k^h - w_{k-1}^h) \right\}_{k=1}^N \right\|_{C_\tau(L_{2h})} \\ & + \left\| \left\{ \frac{p_k + p_{k-1}}{2} \right\}_{k=1}^N \right\|_{C[0,T]_\tau} \left\| \{q_n\}_{n=1}^M \right\|_{L_{2h}}. \end{aligned}$$

Then, the proof of Theorem 1 is based on the following theorem.

Theorem 2. For the solution of DS (6) the stability estimate is satisfied:

$$\begin{aligned} & \left\| \left\{ \frac{1}{\tau} (w_k^h - w_{k-1}^h) \right\}_{k=1}^N \right\|_{C_\tau(L_{2h})} \leq Q_2(a) \left[\|\varphi^h\|_{W_{2h}^2} + |\zeta_0| \right. \\ & \left. + \|f_1^h\|_{L_{2h}} + \left\| \left\{ \frac{1}{\tau} (f_k^h - f_{k-1}^h) \right\}_{k=2}^N \right\|_{C_\tau(L_{2h})} + \left\| \left\{ \frac{\zeta_k - \zeta_{k-1}}{\tau} \right\}_{k=1}^N \right\|_{C[0,T]_\tau} \right]. \end{aligned} \quad (7)$$

Proof. We can write problem (6) as the abstract problem

$$\begin{cases} i \frac{w_k^h - w_{k-1}^h}{\tau} - \frac{A^h}{2} (w_k^h + w_{k-1}^h) = f_k^h + iA^h q^h \frac{\eta_k + \eta_{k-1}}{2}, \\ t_k = k\tau, 1 \leq k \leq N, N\tau = T, w_0^h = \varphi^h \end{cases}$$

in L_{2h} . Then,

$$w_k^h = R^k \varphi^h - i \sum_{j=1}^k R^{k-j} C \tau \left(f_j^h + iA^h q^h \frac{\eta_j + \eta_{j-1}}{2} \right),$$

where

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

Taking the difference derivative and applying the Abel's formula, we get

$$\begin{aligned} \frac{w_k^h - w_{k-1}^h}{\tau} &= -iR^{k-1} C A^h \varphi^h - iC \left(f_1^h + iA^h q^h \frac{\eta_1}{2} \right) \\ &- iC \sum_{j=1}^k R^{k-j} (f_j^h - f_{j-1}^h) + C \sum_{j=1}^k R^{k-j} A^h q^h \frac{\eta_j - \eta_{j-1}}{2}. \end{aligned} \tag{8}$$

Applying formula (8) and estimates

$$\|R\|_{H \rightarrow H} \leq 1, \|C\|_{H \rightarrow H} \leq 1,$$

we get

$$\begin{aligned} \left\| \frac{w_k^h - w_{k-1}^h}{\tau} \right\|_{L_{2h}} &\leq \|A_h^x \varphi^h\|_H + \|f_1^h\|_{L_{2h}} + \sum_{j=2}^k \|f_k^h - f_{k-1}^h\|_{L_{2h}} \\ &+ Q_4(q) \tau \sum_{j=2}^k \left[\left| \frac{\zeta_j - \zeta_{j-1}}{\tau} \right| + \left\| \frac{w_j^h - w_{j-1}^h}{\tau} \right\|_{L_{2h}} \right] \end{aligned}$$

for any k . Then, applying the discrete analogy of the integral inequality, we get

$$\begin{aligned} &\left\| \frac{w_k^h - w_{k-1}^h}{\tau} \right\|_{L_{2h}} \\ &\leq \left[\|A_h^x \varphi^h\|_H + \|f_1^h\|_{L_{2h}} + \sum_{j=2}^k \|f_k^h - f_{k-1}^h\|_{L_{2h}} + Q_4(q) \sum_{j=2}^k |\zeta_j - \zeta_{j-1}| \right] e^{\frac{Q_4(q)k\tau}{1-Q_4(q)\tau}} \end{aligned}$$

for any k . From that it follows (7).

Numerical results

We study the numerical solution of the identification problem

$$\begin{cases} i \frac{\partial u(t,x)}{\partial t} - \frac{\partial^2 u(t,x)}{\partial x^2} + u(t,x) = p(t) (1 + \sin 2x) \\ + (3 \sin(2x) - 1) e^{it}, x \in (0, \pi), t \in (0, 1), \\ u(0, x) = 1 + \sin 2x, x \in [0, \pi], \\ u(t, 0) = u(t, \pi), u_x(t, 0) = u_x(t, \pi), \\ \int_0^\pi u(t, x) dx = \pi e^{it}, t \in [0, 1] \end{cases} \tag{9}$$

for a one dimensional Schrodinger differential equation. The exact solution of this problem is $(u(t, x), p(t)) = ((1 + \sin 2x)e^{it}, e^{it})$. Applying difference scheme (3) for problem (9), we get

$$\left\{ \begin{aligned} & i \frac{u_n^k - u_n^{k-1}}{\tau} - \frac{u_{n+1}^k - 2u_n^k + u_{n-1}^k}{2h^2} - \frac{u_{n+1}^{k-1} - 2u_n^{k-1} + u_{n-1}^{k-1}}{2h^2} + \frac{u_n^k + u_n^{k-1}}{2} \\ & = \frac{p_k + p_{k-1}}{2} (1 + \sin 2x_n) + (3 \sin 2x_n - 1) e^{i(t_k - \frac{\tau}{2})}, \\ & t_k = k\tau, x_n = nh, 1 \leq k \leq N, 1 \leq n \leq M - 1, \\ & u_n^0 = 1 + \sin 2x_n, 0 \leq n \leq M, Mh = \pi, N\tau = 1, \\ & u_M^k = u_0^k, u_M^k - u_{M-1}^k = u_1^k - u_0^k, \\ & \sum_{m=1}^M u_m^k h = \pi e^{it_k}, 0 \leq k \leq N. \end{aligned} \right. \quad (10)$$

The algorithm for obtaining the solution $\{u_n^k\}_0^N$ and $\{p_k\}_1^N$ of DS (10) contains three steps. We introduce η_k by the formula

$$\eta_k = \frac{p_0 + p_k}{2} \tau + \sum_{m=1}^{k-1} p_m \tau, k \in \overline{1, N}, \eta_0 = 0. \quad (11)$$

Then,

$$\frac{p_k + p_{k-1}}{2} = \frac{\eta_k - \eta_{k-1}}{\tau}, k \in \overline{1, N}, \quad (12)$$

$$u_n^k = w_n^k - i\eta_k(1 + \sin 2x_n), k \in \overline{0, N}, n \in \overline{0, M}. \quad (13)$$

Here w_n^k is the solution of the DS

$$\left\{ \begin{aligned} & i \frac{w_n^k - w_n^{k-1}}{\tau} - \frac{w_{n+1}^k - 2w_n^k + w_{n-1}^k}{2h^2} - \frac{w_{n+1}^{k-1} - 2w_n^{k-1} + w_{n-1}^{k-1}}{2h^2} + \frac{w_n^k + w_n^{k-1}}{2} \\ & - z_n h \sum_{k=1}^M w_m^k - z_n h \sum_{k=1}^M w_m^{k-1} = z_n \pi (e^{it_k} + e^{it_{k-1}}) \\ & + (3 \sin 2x_n - 1) e^{i(t_k - \frac{\tau}{2})}, k \in \overline{1, N}, n \in \overline{1, M - 1} \\ & w_n^0 = 1 + \sin 2x_n, n \in \overline{1, M - 1}, \\ & w_M^k = w_0^k, w_M^k - w_{M-1}^k = w_1^k - w_0^k, \end{aligned} \right. \quad (14)$$

where

$$z_n = \frac{1}{\pi + dh} \left[\sin 2x_n \left(\frac{1 - \cos 2h}{h^2} - \frac{1}{2} \right) - \frac{1}{2} \right], n \in \overline{1, M - 1}.$$

Using the discrete analogy of integral condition in (14), we get

$$\eta_k = \frac{\sum_{m=1}^M w_m^k h - \pi e^{it_k}}{i(\pi + dh)}, d = \sum_{m=1}^M \sin 2x_m, k \in \overline{1, N}. \quad (15)$$

Step 1: According to DS (10), we obtain $\{w_n^k\}_0^N$.

We can write (14) as difference equation with matrix coefficients

$$Aw^k + Bw^{k-1} = \varphi^k, 1 \leq k \leq N$$

for any k . Here A and B are $(M + 1) \times (M + 1)$ square matrices and φ is $(M + 1) \times 1$ column matrix

$$A = \begin{bmatrix} 1 & 0 & 0 & \cdot & 0 & -1 \\ a & b - hz_1 & -hz_1 & \cdot & -hz_1 & -hz_1 \\ 0 & a - hz_2 & a - hz_2 & \cdot & -hz_2 & -hz_2 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & -hz_{M-1} & -hz_{M-1} & \cdot & b - hz_{M-1} & a - hz_{M-1} \\ 1 & -1 & 0 & \cdot & -1 & 1 \end{bmatrix}_{(M+1) \times (M+1)},$$

$$B = \begin{bmatrix} 0 & 0 & 0 & \cdot & 0 & 0 \\ a & a - hz_1 & c - hz_1 & \cdot & -hz_1 & 0 \\ 0 & a - hz_2 & c - hz_2 & \cdot & -hz_2 & 0 \\ \cdot & \cdot & \cdot & \cdot & \cdot & \cdot \\ 0 & -hz_{M-1} & -hz_{M-1} & \cdot & c - hz_{M-1} & a \\ 0 & 0 & 0 & \cdot & 0 & 0 \end{bmatrix}_{(M+1) \times (M+1)},$$

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

$$\varphi_n^k = \begin{bmatrix} 0 \\ \varphi_1^k \\ \cdot \\ \varphi_{M-1}^k \\ 0 \end{bmatrix}_{(M+1) \times 1}, w^k = \begin{bmatrix} w_0^k \\ w_1^k \\ \cdot \\ w_{M-1}^k \\ w_M^k \end{bmatrix}_{(M+1) \times 1},$$

$$w^0 = \begin{bmatrix} 1 + \sin 2x_0 \\ 1 + \sin 2x_1 \\ \cdot \\ 1 + \sin 2x_{M-1} \\ 1 + \sin 2x_M \end{bmatrix}_{(M+1) \times 1},$$

$$\varphi_n^k = z_n \pi (e^{it_k} + e^{it_{k-1}}) + (3 \sin 2x_n - 1) e^{i(t_k - \tau/2)}, 1 \leq k \leq N.$$

Therefore

$$w^k = \text{inv}(A) (\varphi^k - Bw^{k-1}).$$

Step 2: We will find $\{\eta_k\}_0^N, \left\{ \frac{p_k + p_{k-1}}{2} \right\}_1^N$ by formulas (12) and (15).

Step 3: We will find $\left\{ \{u_n^k\}_0^N \right\}_0^M$ by formulas (11) and (13). The errors are computed by

$$E_u = \max_{k \in 0, N} \left(\sum_{n=0}^M |u(t_k, x_n) - u_n^k|^2 h \right)^{\frac{1}{2}},$$

$$E_p = \max_{k \in 1, N} \left| p(t_k) - \frac{p_k + p_{k-1}}{2} \right|.$$

Numerical solutions of problem (9) $u(t, x)$ at (t_k, x_n) is u_n^k and of $p(t)$ at t_k is $\frac{p_k + p_{k-1}}{2}$. The result of numerical experience for problem (9) is provided in Table 1.

Table 1

Error Analysis

Error	$M = N = 20$	$M = N = 40$	$M = N = 80$
E_p	0.0002	0.00005	0.00001
E_u	0.017	0.0043	0.0011

Conclusion

In this article the SIP for the one-dimensional SE with non-local boundary conditions is studied. A second order of accuracy Crank-Nicolson difference scheme for the numerical solution of the differential problem is presented. Theorem on stability of this difference scheme is established. The numerical results are given. Finally, this operator approach permits us to investigate one-dimensional SE with classical boundary conditions.

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Дереккөзді идентификациялау бейстационарлы есебі үшін Кранк-Николсонның айырымдық схемасы туралы

Мақалада бейлокалды шекаралық шарттары бар Шредингердің бір өлшемді теңдеуі үшін дереккөзді идентификациялау есебі қарастырылды. Дифференциалдық есепті сандық шешуге арналған екінші дәлдік ретті Кранк-Николсонның айырымдық схемасы ұсынылған. Осы айырымдық схеманың шешімінің тұрақтылығын бағалаулары дәлелденді және сандық нәтижелер келтірілген.

Кілт сөздер: идентификациялау мәселесі, Шредингер теңдеуі, айырымдық схемасы, Кранк-Николсон, тұрақтылық.

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О разностной схеме Кранка-Николсона для нестационарной задачи идентификации источника

В статье рассмотрена задача идентификации источника для одномерного уравнения Шредингера с нелокальными граничными условиями. Представлена разностная схема Кранка-Николсона второго порядка точности для численного решения дифференциальной задачи. Доказаны оценки устойчивости решения этой разностной схемы, и приведены численные результаты.

Ключевые слова: проблема идентификации, уравнение Шредингера, разностная схема Кранка-Николсона, устойчивость.

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