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Abstract

This paper presents a numerical solution of an optimal control problem for linear parabolic equations. The estimates for the error of the difference scheme and the speed of convergence have been established. Numerical results are reported on test problems.

Key Words: Optimal control problem, Finite difference method, Inverse problem

1. Introduction and Statement of the Problem

Many theoretical phenomena which are governed by linear and nonlinear parabolic equations have been investigated in the field of optimal control. Many problems in theoretical physics, for example [1], [2], [3], [4], can be expanded to these types of problems. Also, determining the quantum-mechanical potential is one of the basic problems of the quantum mechanics. Given simplifying assumptions, this potential is determined on the basis of intuitive concepts [1]. Problems of determining interaction potentials have stimulated the development of scattering theory [1]. Different approaches for solving optimal control problems of parabolic systems and inverse problems were proposed in [8], [10],

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[11], [12] and numerical solutions of Schrödinger equations were investigated in [9], [16]. In many applications as in the quantum-mechanical, heat equation and hydrology there is a need to recover control coefficient v from boundary measurements of solutions of a parabolic equations. The inverse problem of determining the quantum-mechanical potential is not well-posed, and this also holds in the variational formulation, so it is quite difficult to obtain numerical solution. In the variational formulation, an optimal control of the coefficient, that is, of the potential in the Schrodinger equation, is produced [13].

The paper is organized as follows. First, differences scheme and its error are evaluated in Section 2. Second, convergence speed of the difference approximations is examined and some estimates are obtained. Finally, in Section 4, a minimization algorithm is given for the optimal control problem and this algorithm is tested in two quantum mechanical problems.

Let Ω region be $\Omega = (0,l) \times (0,T)$, $T > 0$ a specified number, $0 \leq t \leq T$. Let the spaces $W_p^k(0,l)$ and $W_p^{k,m}(\Omega)$, $p \geq 1$, k, $m \geq 0$ be defined as in [5], and symbol $\overset{\circ}{\forall}$ signify that the given property applied for almost all values of variable quantity.

We consider a quantum-mechanical system whose state described by the Schrödinger equation

$$i\frac{\partial \psi}{\partial t} + a_0 \frac{\partial^2 \psi}{\partial x^2} - v\left(x\right)\psi = f\left(x,t\right), \quad (x,t) \in \Omega, \tag{1}$$

where $\psi = \psi(x,t)$ is a wave function, $i = \sqrt{-1}$, a is a specified positive number, $f \in W_2^{2,0}(\Omega)$. Let the following initial and boundary conditions be specified for (1):

$$\psi\left(x,0\right) = \phi\left(x\right), \quad x \in (0,l) \tag{2}$$

$$\frac{\partial \psi(0,t)}{\partial x} = \frac{\partial \psi(l,t)}{\partial x} = 0, \; t \in (0,T), \tag{3}$$

where $\varphi(x)$ is a given function from $W_2^3(0,l)$ and φ and f satisfy the conditions,

$$\frac{d\varphi(0)}{dx} = \frac{d\varphi(l)}{dx} = 0, \tag{4}$$

$$\frac{\partial f\,(0,t)}{\partial x} = \frac{\partial f\,(l,t)}{\partial x} = 0, \frac{\partial f}{\partial t} \in W_2^{1,0}\,(\Omega) \tag{5}$$

respectively. Our aim is to determine the potential $v(x)$ on the basis of additional information $\psi(x,T) = y(x)$ concerning the solution of (1) under conditions (2)-(3). We will look for the function $v(x)$ in the set

$$V = \left\{ v : v = v\,(x)\,,\, v \in L_2\,(0,l)\,,\, b_0 \leq v\,(x) \leq b_1,\,,\, \overset{\circ}{\forall}\, x \in (0,l) \right\},$$

(where $b_0 \geq 0$ and $b_1 \geq 0$ are given number), called the class of admissible potentials.

Suppose that $J_0(v)$ is defined as

$$J_0(v) = \int_0^l |\psi(x,T;v) - y(x)|^2.$$

Therefore, the variational formulation of this problem requires in minimizing the functional

$$J_\alpha(v) = J_0(v) + \alpha||v-w||^2_{L_2(0,l)} \tag{6}$$

in the set V, where $\alpha > 0$ is a given number, $y \in W_2^1(0,l)$, $w \in L_2\,(0,l)$ are given functions. The second term in the right hand side of (6) is introduced with aim of a further possible regularization of the initial problem [7].

By a solution of problem (1)-(2) with a given $v \in V$ (this problem is a boundary value problem for (1), we call it as the reduced problem), we will understand a function $\psi(x,t)$ belongs to the space $W_2^{2,1}(\Omega)$ and satisfies

$$\int_\Omega (-i\eta_t + a_0\eta_{xx} - v(x)\eta)\,\psi\,dx\,dt = \int_\Omega f(x,t)\eta(x,t)\,dxdt$$
$$+\,i\int_0^l \eta(x,0)\varphi(x)\,dx + \int_0^T \psi(l,t)\eta_x(l,t)\,dt - \int_0^T \psi(0,t)\eta_x(0,t)\,dt$$

for any $\eta = \eta(x,t) \in W_2^{2,1}(\Omega)$ and any $t \in [0,T]$.

We note that the reduced problem has been investigated in [5], [6] and elsewhere. The results obtained there are, however of little use for our purposes, since in them the potentials are assumed to be sufficiently smooth even for non smooth solutions of the Schrödinger equation. As the solution of the reduced problem (1)-(3) explicitly depends on the control v, we shall therefore also use the notation $\psi = \psi(x,t;v)$.

Existence and uniqueness of the solution (1)-(3), (6) have been investigated in [15]In this study we especially show how a finite difference scheme can be used to solve this problem, and give estimates on the rate of convergence. We prove that the minimum of the (discrete) cost functional for an approximate optimal control problem converges to the minimum of the cost functional of the original problem as the grid spacing tends to zero.

2. Differences Scheme and Its Error

In this section, we shall use finite-difference method for the solution of the problem (1)-(3), (6). For the various partial derivatives of the function $\phi(x,t)$ let us write the difference quotients and discretization scheme:

$$\{(x_j, t_k)_n\},\ n = 1, 2, \ldots, \qquad j = \overline{0, M_n}, \qquad k = \overline{0,\ N_n}$$

$$x_j = jh - \frac{h}{2}, \quad t_k = k\tau, \quad h = h_n = \frac{l}{(M_n - 1)}, \ \tau = \tau_n = \frac{T}{N_n}.$$

$$M = M_n,\ N = N_n, \quad \delta_{\overline{t}}\phi_{j\quad k} = \frac{(\phi_{jk} - \phi_{jk-1})}{\tau}$$

$$\delta_x \phi_{jk} = \frac{(\phi_{j+1\,k} - \phi_{jk})}{h}, \quad \delta_{x\overline{x}}\phi_{jk} = \frac{(\delta_x\phi_{jk} - \delta_{\overline{x}}\phi_{jk})}{h}.$$

For arbitrary natural number $m \geq 1$, let us consider the minimizing problem of the functional

$$I_m([v]_m) = h \sum_{j=1}^{M-1} |\phi_{jN} - y_j|^2 \tag{7}$$

in the set $V_m = \{[v]_m : [v]_m = (v_1, v_2, \ldots, v_{M-1}),\ |v_j| \leq b_0,\ j = \overline{1, M-1}\,\}$ under the conditions

$$i\delta_{\overline{t}}\phi_{jk} + a_0\delta_{x\overline{x}}\phi_{jk} - v_j\phi_{jk} = f_{jk},\ \ j = \overline{1, M-1},\ \ k = \overline{1, N}, \tag{8}$$

$$\phi_{j0} = \varphi_j, \quad j = \overline{0, M}, \tag{9}$$

$$\delta_{\overline{x}}\phi_{1k} = \delta_{\overline{x}}\phi_{Mk} = 0, \quad k = \overline{1, N}, \tag{10}$$

where $y_j,\ \varphi_j,\ f_{jk}$ scheme functions are determined by

$$y_j = \frac{1}{h}\int_{x_j-h/2}^{x_j+h/2} y(x)\,dx$$

$$\varphi_j = \frac{1}{h}\int_{x_j-h/2}^{x_j+h/2} \varphi(x)\,dx,\ \ j = \overline{1,\, M-1},\ \ \varphi_0 = \varphi_1,\ \ \varphi_M = \varphi_{M-1}$$

$$f_{jk} = \frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2} f(x,t)\,dxdt, \quad j = \overline{1,\, M-1}, \quad k = \overline{1, N}$$

respectively. Using additive identities and the method of a priori estimates, we write the estimate

$$h\sum_{j=1}^{M-1} |\phi_{jn}|^2 \leq c_5\left(h\sum_{j=1}^{M-1}|\varphi_j|^2 + \tau h\sum_{k=1}^{N}\sum_{j=1}^{M-1}|f_{jk}|^2\right),\ \forall n \in \{1, 2, 3, \ldots, N\} \tag{11}$$

for the solution of differences scheme (8)-(10), where $c_5 > 0$ is a constant that does not depend on τ and h. Now, we will evaluate the error of the differences scheme (8)-(10). For this purpose let us consider the following system:

$$i\delta_{\overline{t}}z_{jk} + a_0\delta_{x\overline{x}}z_{jk} - v_jz_{jk} = F_{jk},\ j = \overline{1,\, M-1},\ k = \overline{1, N}, \tag{12}$$

$$z_{j0} = 0, \quad j = \overline{0, M}, \quad \delta_{\overline{x}} z_{1k} = \delta_{\overline{x}} z_{Mk} = 0, \quad k = \overline{1, N}, \tag{13}$$

where $z_{jk} = \phi_{jk} - \psi_{jk}$, $\{\phi_{jk}\}$ is the solution of the system (8)-(10), $\{\psi_{jk}\}$ is determined by

$$\psi_{jk} = \frac{1}{h} \int_{x_j - h/2}^{x_j + h/2} \psi(x, t_k) dx, \quad j = \overline{1, M-1}, \quad k = \overline{1, N},$$

$$\psi_{j0} = \varphi_j, \;\; j = \overline{0, M}, \quad \psi_{0k} = \psi_{1k}, \psi_{Mk} = \psi_{M-1\,k}, \quad k = \overline{1, N},$$

and the scheme functions F_{jk} is defined by

$$F_{jk} = \frac{1}{\tau h} \int_{t_{k-1}}^{t_k} \int_{x_j - h/2}^{x_j + h/2} \left(i \frac{\partial \psi}{\partial t} + a_0 \frac{\partial^2 \psi}{\partial x^2} - v(x) \psi \right) dx\, dt - i \delta_{\overline{t}} \psi_{jk} - \tag{14}$$

$$- a_0 \delta_{x\overline{x}} \psi_{jk} + v^j \psi_{jk}, \quad j = \overline{1,\, M-1}, \quad k = \overline{1,\, N}.$$

Let us define the operator Q_m by

$$Q_m(v) = \left(v^1, v^2, \dots, v^{M-1} \right), \quad v^j = \frac{1}{h} \int_{x_j - h/2}^{x_j + h/2} v(x) dx, \quad j = \overline{1,\, M-1} \tag{15}$$

in the set V. Therefore we can write the following theorem.

Theorem 1 *Suppose that the steps $\tau > 0$ and $h > 0$ satisfy the compatibility condition $c_6 \le \frac{\tau^2}{h^2} \le c_7$, where $c_6, c_7 > 0$ are constants independent from τ and h. Therefore, the estimate*

$$h \sum_{j=1}^{M-1} |z_{jn}|^2 \le c_8 \left(\tau^2 + h^2 + ||Q_m(v) - [v]_m||^2 \right), \quad \forall n \in \{1, 2, \dots, N\}, \tag{16}$$

is valid, where $c_8 > 0$ is a constant that does not depend on τ and h.

Proof. We obtain the estimate

$$h\sum_{j=1}^{M-1}|z_{jn}|^2 \quad \leq c_9\left(\tau h\sum_{k=1}^{N}\sum_{j=1}^{M-1}|F_{jk}|^2\right), \quad \forall n\in\{1,2,\dots N\}, \tag{17}$$

as similar way for the estimate (11), by using additive identities for the solution of system (12)-(13), where $c_9>0$ is a constant that does not depend on τ and h.

Now, let us evaluate the right hand side of the estimate (17). According to (14), we obtain

$$F_{jk}=F_{jk}^1+F_{jk}^2+F_{jk}^3, \quad j=\overline{M-1},\ k=\overline{1,N}, \tag{18}$$

where

$$F_{jk}^1=\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2} i\frac{\partial\psi}{\partial t}dxdt-i\delta_{\overline{t}}\psi_{jk}, \tag{19}$$

$$F_{jk}^2=\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2} a_0\frac{\partial^2\psi}{\partial x^2}dxdt-a_0\delta_{x\overline{x}}\psi_{jk}, \tag{20}$$

$$F_{jk}^3=v^j\psi_{jk}-\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2} v\psi\, dxdt. \tag{21}$$

From (19) and definition of the scheme functions ψ_{jk}, we obtain

$$F_{jk}^1=0, \quad j=\overline{1,\,M-1}, \quad k=\overline{1,N}. \tag{22}$$

From (20) and the formula for ψ_{jk}, we obtain

$$\begin{aligned}
F_{jk}^{2} =& \frac{a_0}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\frac{\partial^2\psi(x,t)}{\partial x^2}\,dx\,dt - \frac{a_0}{h^2}\bigg\{\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_{j+1}-h/2}^{x_{j+1}+h/2}\psi(x,t)dxdt\\
&-\frac{2}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\psi(x,t)\,dxdt + \frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\psi(x,t)\,dxdt\bigg\}\\
&-\frac{a_0}{h^2}\bigg\{\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_{j+1}-h/2}^{x_{j+1}+h/2}(\psi(x,t_k)-\psi(x,t))dxdt\\
&-\frac{2}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}(\psi(x,t_k)-\psi(x,t))dxdt\\
&+\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_{j-1}-h/2}^{x_{j-1}+h/2}(\psi(x,t_k)-\psi(x,t))dxdt\bigg\}\\
&= F_{jk}^{21}+F_{jk}^{22}, \qquad j=\overline{2,M}-2,\;\; k=\overline{1,N}. \qquad (23)
\end{aligned}$$

where

$$\begin{aligned}
F_{jk}^{21} =& \frac{a_0}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\frac{\partial^2\psi(x,t)}{\partial x^2}\,dx\,dt - \frac{a_0}{h^2}\bigg\{\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_{j+1}-h/2}^{x_{j+1}+h/2}\psi(x,t)dxdt\\
&-\frac{2}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\psi(x,t)\,dxdt + \frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\psi(x,t)\,dxdt\bigg\}
\end{aligned}$$

and

$$\begin{aligned}
F_{jk}^{22} =& -\frac{a_0}{h^2}\bigg\{\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_{j+1}-h/2}^{x_{j+1}+h/2}(\psi(x,t_k)-\psi(x,t))dxdt\\
&-\frac{2}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}(\psi(x,t_k)-\psi(x,t))dxdt\\
&+\frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_{j-1}-h/2}^{x_{j-1}+h/2}(\psi(x,t_k)-\psi(x,t))dxdt\bigg\}.
\end{aligned}$$

By using formula of F_{jk}^{22} in (23), we write

$$F_{jk}^{22}=-\frac{a_0}{\tau h^3}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\int_t^{t_k}\int_{x-h}^{x}\left(\frac{\partial^2\psi(\xi+h,\theta)}{\partial\xi\partial\theta}-\frac{\partial^2\psi(\xi,\theta)}{\partial\xi\partial\theta}\right)d\xi d\theta dx dt, \qquad (24)$$

where $j=\overline{2,M-2},\ k=\overline{1,N}$. Hence we obtain

$$\left|F_{jk}^{22}\right|\leq\frac{a_0\tau^{\frac{1}{2}}}{h^{3/2}}\left(\int_{t_{k-1}}^{t_k}\left\{\int_{x_j-h/2}^{x_j+h/2}\left|\frac{\partial^2\psi(x+h,t)}{\partial x\partial t}-\frac{\partial^2\psi(x,t)}{\partial x\partial t}\right|^2 dx\right.\right. \qquad (25)$$

$$\left.\left.+\int_{x_{j-1}-h/2}^{x_{j-1}+h/2}\left|\frac{\partial^2\psi(x+h,t)}{\partial x\partial t}-\frac{\partial^2\psi(x,t)}{\partial x\partial t}\right|^2 dx\right\}dt\right)^{1/2},\ j=\overline{2,M-2},\ k=\overline{1,N}$$

By using the formula of F_{jk}^{21} in (23), we write

$$F_{jk}^{21}=\frac{a_0}{\tau}\int_{t_{k-1}}^{t_k}\left\{\frac{1}{h}\left(\frac{\partial\psi(x_j+h/2,t)}{\partial x}-\frac{\partial\psi(x_j-h/2,t)}{\partial x}\right)\right. \qquad (26)$$

$$-\frac{1}{h^3}\left(\int_{x_{j+1}-h/2}^{x_{j+1}+h/2}\psi(x,t)dx-2\int_{x_j-h/2}^{x_j+h/2}\psi(x,t)\,dx\right.$$

$$\left.\left.+\int_{x_{j-1}-h/2}^{x_{j-1}+h/2}\psi(x,t)dx\right)\right\}dt$$

for $j=\overline{2,M-2},\ k=\overline{1,N}$. Suppose that

$$P_t(\psi)=\frac{1}{h}\left(\frac{\partial\psi(x_j+h/2,t)}{\partial x}-\frac{\partial\psi(x_j-h/2,t)}{\partial x}\right) \qquad (27)$$

$$-\frac{1}{h^3}\left(\int_{x_{j+1}-h/2}^{x_{j+1}+h/2}\psi(x,t)dx-2\int_{x_j-h/2}^{x_j+h/2}\psi(x,t)\,dx+\int_{x_{j-1}-h/2}^{x_{j-1}+h/2}\psi(x,t)dx\right)$$

Now, let us replace the variable x_j with x and the variable x with ξ and take $\xi=x+sh$. Therefore $P_t(\psi)$ is written as

$$P_t(\widetilde{\psi})=\frac{1}{h^2}\left\{\left(\frac{\partial\widetilde{\psi}(0.5,t)}{\partial s}-\frac{\partial\widetilde{\psi}(-0.5,t)}{\partial s}\right)\right.$$

$$- \int_{0.5}^{1.5} \widetilde{\psi}(s,t)ds + 2\int_{-0.5}^{0.5} \widetilde{\psi}(s,t)\,ds - \int_{-1.5}^{-0.5} \widetilde{\psi}(s,t)ds \Big\}, \tag{28}$$

where $\widetilde{\psi}(s,t) = \psi(x+sh,t)$. It is obvious that the functional $P_t(\widetilde{\psi})$ is linear according to $\widetilde{\psi}$. Moreover, the functional is bounded in the space $W_2^3(-0.5,\,0.5)$. Therefore, we write

$$|P_t(\widetilde{\psi})| \leq c_{10}h^{-2}||\widetilde{\psi}||_{W_2^3(-0.5,0.5)},\ \overset{\circ}{\forall}\ t \in (0,T) \tag{29}$$

by using (28), where $c_{10} > 0$ is a constant that does not depend on τ and h. It can be easily shown that the functional $P_t(\widetilde{\psi})$ is zero at $\widetilde{\psi} = as^2 + bs + c$, that is

$$P_t(\widetilde{\psi}) = P_t(as^2 + bs + c) = 0.$$

Hence, the conditions of the Bramble-Hilbert Lemma hold [10]. Therefore, we obtain

$$\left|P_t(\widetilde{\psi})\right| \leq c_{11}h^{-2}\Big|\Big|\frac{\partial^3\widetilde{\psi}}{\partial s^3}\Big|\Big|_{L_2(-0.5,0.5)},\quad \overset{\circ}{\forall}\ t \in (0,T) \tag{30}$$

from hypothesis of this Lemma and estimate (29). Now, by reversing variables and using (26), (27), (30) and first assignments, we write

$$\left|F_{jk}^{21}\right| \leq c_{11}h^{1/2}\tau^{-1/2}\left(\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2}\left|\frac{\partial^3\psi}{\partial x^3}\right|^2 dxdt\right)^{1/2},\ j=\overline{2,M-2},\ k=\overline{1,N}\ . \tag{31}$$

If we use the formulas of F_{1k}^2, $F_{M-1\,k}^2$ and the conditions

$$\frac{\partial\psi(0,t)}{\partial x} = \frac{\partial\psi(x_1-h/2,t)}{\partial x} = \frac{\partial\psi(l,t)}{\partial x} = \frac{\partial\psi(x_{M-1}+h/2,t)}{\partial x} = 0,$$

then we prove the inequalities

$$\left|F_{1k}^2\right| \leq \frac{a_0\tau^{1/2}}{h^{3/2}}\left(\int_{t_{k-1}}^{t_k}\left\{\int_{x_1-h/2}^{x_1+h/2}\left|\frac{\partial^2\psi(x,t)}{\partial x\partial t}\right|^2 dx + \int_{x_2-h/2}^{x_2+h/2}\left|\frac{\partial^2\psi(x,t)}{\partial x\partial t}\right|^2 dx\right\}dt\right)^{1/2} +$$

$$+c_{12}a_0h^{1/2}\tau^{-1/2}\left(\int_{t_{k-1}}^{t_k}\int_{x_1-h/2}^{x_1+h/2}\left|\frac{\partial^3\psi(x,t)}{\partial x^3}\right|^2 dxdt\right)^{1/2}, \tag{32}$$

$$\left|F_{M-1k}^2\right| \le \frac{a_0\tau^{1/2}}{h^{3/2}}\left(\int_{t_{k-1}}^{t_k}\left\{\int_{x_{M-2}-h/2}^{x_{M-2}+h/2}\left|\frac{\partial^2\psi(x,t)}{\partial x\partial t}\right|^2 dx+\right.\right.$$

$$\left.\left.+\int_{x_{M-1}-h/2}^{x_{M-1}+h/2}\left|\frac{\partial^2\psi(x,t)}{\partial x\partial t}\right|^2 dx\right\}dt\right)^{1/2} + c_{13}a_0h^{1/2}\tau^{-1/2}\times$$

$$\times\left(\int_{t_{k-1}}^{t_k}\int_{x_{M-1}-h/2}^{x_{M-1}+h/2}\left|\frac{\partial^3\psi(x,t)}{\partial x^3}\right|^2 dxdt\right)^{1/2} \tag{33}$$

according to the Bramble-Hilbert lemma, where $c_{12}, c_{13} > 0$ are constants independent from τ and h. Hence, from inequalities (27), (33), formula (25) and compatible condition, we obtain

$$\tau h\sum_{k=1}^{N}\sum_{j=1}^{M-1}\left|F_{jk}^2\right|^2 \le c_{14}h^2\left(\left|\left|\frac{\partial^3\psi}{\partial x^3}\right|\right|_{L_2(\Omega)}^2 + \left|\left|\frac{\partial^2\psi}{\partial x\partial t}\right|\right|_{L_2(\Omega)}^2\right), \tag{34}$$

where $c_{14} > 0$ is a constant independent from h and τ. In the statement of

$$F_{jk} = \frac{1}{\tau h}\int_{t_{k-1}}^{t_k}\int_{x_j-h/2}^{x_j+h/2} v(x)\left(\psi_{jk} - \psi(x,t)\right)dxdt, \tag{35}$$

using by formula of ψ_{jk}, we can also write equality

$$\psi_{jk} - \psi(x,t) = \frac{1}{h}\int_{x_j-h/2}^{x_j+h/2}\left\{\int_t^{t_k}\frac{\partial\psi(\xi,\theta)}{\partial\theta}d\theta + \int_x^{\xi}\frac{\partial\psi(\eta,t)}{\partial\eta}d\eta\right\}d\xi. \tag{36}$$

Then we obtain the inequality

$$\tau h \sum_{k=1}^{N} \sum_{j=1}^{M-1} \left| F_{jk} \right|^2 \leq c_{15}(\tau^2 + h^2) \left(\left|\left| \frac{\partial \psi}{\partial t} \right|\right|^2_{L_2(\Omega)} + \left|\left| \frac{\partial \psi}{\partial x} \right|\right|^2_{L_2(\Omega)} \right), \tag{37}$$

where $c_{15} > 0$ is a constant independent from h and τ. Hence, we write

$$F^3_{jk} = \frac{\psi_{jk}}{h} \int_{x_j-h/2}^{x_j+h/2} \left(v^j - v(x) \right) dx + \frac{1}{\tau h} \int_{t_{k-1}}^{t_k} \int_{x_j-h/2}^{x_j+h/2} v(x) \left(\psi_{jk} - \psi(x,t) \right) dx dt \tag{38}$$

for $j = \overline{1, M-1}$, $k = \overline{1, N}$. By using formula of ψ_{jk} and the estimate (8), we prove the estimate

$$\left| \psi_{jk} \right| \leq c_{16}, \;\; j = \overline{1, M-1}, \;\; k = \overline{1, N}, \tag{39}$$

where $c_{16} > 0$ is constant independent from h and τ. Therefore, if we consider equality (36) and inequality (37), then we obtain □

$$\tau h \sum_{k=1}^{N} \sum_{j=1}^{M-1} \left| F^3_{jk} \right|^2 \leq c_{15} \left\{ (\tau^2 + h^2) \left(\left|\left| \frac{\partial \psi}{\partial t} \right|\right|^2_{L_2(\Omega)} + \left|\left| \frac{\partial \psi}{\partial x} \right|\right|^2_{L_2(\Omega)} \right) + ||Q_m(v) - [v]_m||^2 \right\} \tag{40}$$

from (38). Hence, by using inequality (34) and equalities (38) and (22), We show that the hypothesis of the theorem is true. The proof is completed.

3. Convergence of the Difference Approximations

Now, let us evaluate the difference between original functional and discrete functional.

Theorem 2 *Suppose that the conditions of Theorem 1 hold. Then the estimate*

$$|J(v) - I_m([v]_m)| \leq c_{18}(\tau + h + ||Q_m(v) - [v]_m||) \tag{41}$$

is valid for $\forall v \in V$ *and* $\forall [v]_m \in V_m$*, where* $c_{18} > 0$ *is a constant independent from* h *and* τ*.*

Proof. By using the formulas of functional, we write the difference between them as

$$J(v) - I_m([v]_m) = \sum_{j=1}^{M-1} \int_{x_j - h/2}^{x_j + h/2} \Big\{ |\psi(x,T) - y(x)|^2 - |\phi_{jN} - y_j|^2 \Big\} dx. \tag{42}$$

If we apply Cauchy-Bunyakowski inequality and use (7) , then we write

$$\Big| J(v) - I_m([v]_m) \Big| \le c_{19} \Bigg\{ \Bigg(\sum_{j=1}^{M-1} \int_{x_j - h/2}^{x_j + h/2} |\psi(x,T) - \phi_{jN}|^2 dx \Bigg)^{1/2} +$$

$$+ \Bigg(\sum_{j=1}^{M-1} \int_{x_j - h/2}^{x_j + h/2} |y - y_j|^2 dx \Bigg)^{1/2} \Bigg\} = c_{19} \{ J_1 + J_2 \} \tag{43}$$

from (42), where

$$J_1 = \Bigg(\sum_{j=1}^{M-1} \int_{x_j - h/2}^{x_j + h/2} |\psi(x,T) - \phi_{jN}|^2 dx \Bigg)^{1/2}$$

and

$$J_2 = \Bigg(\sum_{j=1}^{M-1} \int_{x_j - h/2}^{x_j + h/2} |y - y_j|^2 dx \Bigg)^{1/2}.$$

Since $y \in W_2^1(0,l)$, we can write

$$J_2 \le h \Big\| \frac{\partial y}{\partial x} \Big\|_{L_2(0,l)}. \tag{44}$$

By using the formula of J_1, we obtain

$$J_1 \leq \sqrt{2}\Big\{ \sum_{j=1}^{M-1} \int_{x_j-h/2}^{x_j+h/2} |\psi(x,T) - \psi_{jN}|^2 dx +$$

$$+h \sum_{j=1}^{M-1} |\psi_{jN} - \phi_{jN}|^2 \Big\}^{1/2} = \sqrt{2}\{J_1^1 + J_1^2\}^{1/2}, \tag{45}$$

where $n = N$. From the estimate (17), we write

$$J_1^2 \leq c_{20}(\tau^2 + h^2 + ||Q_m(v) - [v]_m||^2). \tag{46}$$

Using formula of the ψ_{jk}, we have

$$J_1^1 \leq \sum_{j=1}^{M-1} \int_{x_j-h/2}^{x_j+h/2} \Big| \int_{x_j-h/2}^{x_j+h/2} \int_x^{\xi} \frac{\partial\psi(\eta,T)}{\partial\eta} \mathrm{d}\eta d\xi \Big|^2 dx.$$

Therefore, from the inequality

$$\Big|\Big|\frac{\partial\psi(.,T)}{\partial x}\Big|\Big|_{L_2(0,l)} \leq c_{21}\left(\Big|\Big|\frac{\partial\psi}{\partial x}\Big|\Big|_{L_2(\Omega)} + \Big|\Big|\frac{\partial^2\psi}{\partial x \partial t}\Big|\Big|_{L_2(\Omega)}\right)$$

and estimate (8), we obtain

$$J_1^1 \leq c_{22}h. \tag{47}$$

Hence, according to inequalities (46), (47) , we obtain

$$J_1 \leq c_{23}(\tau + h + ||Q_m(v) - [v]_m||). \tag{48}$$

Consequently, in view of (44) and (48) the hypothesis of the Theorem 2 holds.

Now, let us obtain an estimate for convergence speed of difference approximations according to functional. For this purpose, we write the following lemmas. □

Lemma 1 *Suppose that the conditions of Theorem 2 hold, and the operator* Q_m *is defined by (15). Then* $Q_m(v) \in V$*, and the following the estimate*

$$|J(v) - I_m(Q_m(v)| \leq c_{24}(\tau + h). \tag{49}$$

is valid, where $c_{24} > 0$ *is a constant that does not depend on* h *and* τ*.*

Proof. Suppose that $v \in V$ is an arbitrary function. Therefore, we can write that $Q_m : V \to V_m$ from definition of the sets V_m and Q_m. Consequently, if we take $Q_m(v)$ instead of discrete function V_m in Theorem 2 then we obtain the estimate (49). Hence, this Lemma is proved. □

Lemma 2 *Suppose that conditions of Theorem 2 hold and the operator* P_m *is defined by*

$$P_m([v]_m) = \widetilde{v}(x), \;\; \widetilde{v}(x) = v_j, \;\; x_j - h/2 \leq x \leq x_j + h/2, \quad j = \overline{1, M-1}.$$

Therefore $P_m([v]_m) \in V$ *and*

$$|J(P_m([v]_m)) - I_m([v]_m)| \leq c_{25}(\tau + h), \tag{50}$$

where $c_{25} > 0$ *is a constant that does not depend on* h *and* τ*.*

Proof. Suppose that $[v_m] \in V_m$ is a arbitrary discrete function. From definition of the set V and the operator $P_m([v]_m)$ we write $P_m : V_m \to V$. Therefore, if we take $P_m([v_m])$ instead of v in Theorem 2 then we obtain the estimate (50) considering (43). Hence, this Lemma is proved. □

Theorem 3 *Suppose that the conditions of Lemma 1 and Lemma 2 hold and let* $v^* \in V$, $[v]_m^* \in V_m^*$ *be are solutions of the problems (1)-(3) and (7)-(10) respectively, that is,*

$$J_* = \inf_{v \in V} J(v) = J(v^*), \quad I_{m*} = \inf_{[v]_m \in V_m} I_m([v]_m) = I_m([v]_m^*).$$

Therefore the solutions of the problem (7)-(10) are approximate to solution of the problem (1)-(3). That is

$$\lim_{m \to \infty} I_{m*} = J_*$$

and the estimate

$$|I_{m*} - J_*| \leq c_{26}(\tau + h) \tag{51}$$

is true for the convergence speed of the difference approximations, where $c_{26} > 0$ *is a constant that does not depend on* h *and* τ*.*

Proof. Let us consider (49) again. It can be easily seen that τ and h are sufficiently small for increasing m. We have $J(v) = I_m([v]_m)$, for $m \to \infty$. Also, in the cases $J_* = \inf_{v \in V} J(v)$ and $I_{m*} = \inf_{[v]_m \in V_m} I_m([v]_m)$, the statement

$$\lim_{m \to \infty} I_{m*} = J_*$$

holds and when we consider the infimum status of (50), the estimate (51) holds. □

4. Numerical Solution of the Optimal Control Problem

In this section we will give an algorthim for the solution of the problem (1)-(3), (6). This problem is an invers problem and it is ill-posed. In Theorem 1, we showed that this problem has at least one solution. Since the problem (1)-(3), (6) is ill-posed we use Tikhonov method [7] for the solution of the problem. We need a stabilizator function while using this method. Suppose that the stabilizator function is defined as

$$S(v) = ||v - w||^2_{L_2(\Omega)} = \int_0^T \int_0^l |v(x,t) - w(x,t)| \, dx \, dt$$

in the set V, where $w(x,t) \in L_2(\Omega)$ is a given function. It can be shown that $S(v)$ is a stabilazator [14]. Let us take a sequence $\{\alpha^m\}$ having property that $\{\alpha^m\} \to 0$ at $m \to \infty$. Also, let us define the functional

$$J_m(v) = J_\alpha(v) + \alpha^m S(v),\ v \in V \tag{52}$$

in the set V for the each $m = 1, 2, \ldots ,$. Now, we will investigate the minimizing problem for the functional $J_m(v)$ under the conditions (1)-(3). Firstly, we will write discretization of this problem. Let us consider a grid in the plane xt. We divide [0,l] into M and $[0,T]$ into N equal subintervals with the constant steps h and τ respectively. Where $h = l/M$ and $\tau = T/N$. Therefore the mesh points in the x axis are

$$[x_0, x_1],\ \ldots\ ,\ [x_0 + (M-1)h,\ x_0 + Mh],\ x_j = x_0 + jh,\ j = \overline{0, M}$$

and mesh points in the t axis are

$$[t_0, t_1], \ldots , [t_0 + (N-1)\tau,\ t_0 + N\tau],\ t_k = t_0 + k\tau,\ k = \overline{1, N}$$

Let us choose the set V_M as discretization of the admisible controls set V. We can write the V_M as follows

$$V_M = \{[v],\ [v] = v_j,\ j = 0, M,\ \ 0 < b_0 \le v_j \le b_1\}.$$

Hence discretization of the problem

$$J_m(v) \to \min$$

can be written as

$$I_m(v) \to \min \tag{53}$$

in the set V_M under the conditions

$$i\delta_t \phi_{jk} - a_0 \delta_{\overline{x}x} \phi_{jk} - v_j \phi_{jk} = f_{jk},\ j = \overline{1, M-1},\ \ k = \overline{1, N} \tag{54}$$

$$\phi_{j0} = \varphi_j,\ j = \overline{0, M} \tag{55}$$

$$\delta_x \phi_{0k} = \frac{h}{2a_0} \left(f_{0k} - i\delta_{\overline{t}}\phi_{0k} - v_0\phi_{0k} \right),\ \ k = \overline{1, N} \tag{56}$$

$$\delta_x \phi_{Mk} = \frac{h}{2a_0} \left(f_{Mk} - i\delta_{\overline{t}}\phi_{Mk} - v_M\phi_{Mk} \right),\ \ k = \overline{1, N}, \tag{57}$$

where

$$I_m(v) = h \sum_{j=1}^{M-1} |\phi_{jN} - y_j|^2 + \tag{58}$$

$$\alpha^m \tau \sum_{k=1}^{N} \left(\sum_{j=1}^{M-1} |v_j - w_j|^2 + \frac{1}{2}|v_0 - w_0|^2 + |v_M - w_M|^2 \right),$$

$f_{jk} = f(x_j, x_k)$, $w_{jk} = w(x_j, t_k)$, $\varphi_j = \varphi(x_j)$, $j = \overline{0, M}$, $k = \overline{1, N}$.

We will use projection of the gradient method for the solution of the problem (53)-(57), for this purpose we can write the gradient of the discrete function as

$$(I'_m([v]))_{jk} = -Re(\phi_{jk}\overline{\eta}_{jk}) + 2\alpha^m(v_j - w_j),\ j = \overline{0, M-1},\ \ k = \overline{1, N}$$

where η is the solution of the problem

$$i\delta_t \eta_{jk} - a_0 \delta_{\overline{x}x}\eta_{jk} - v_j\eta_{jk} = f_{jk},\ j = \overline{1, M-1},\ \ k = \overline{1, N} \tag{59}$$

$$\eta_{jN} = \varphi_j,\ j = \overline{0, M} \tag{60}$$

$$\delta_x \eta_{0k} = \frac{h}{2a_0} \left(f_{0k} - i\delta_{\overline{t}}\eta_{0k} - v_0\eta_{0k} \right),\ \ k = \overline{1, N} \tag{61}$$

$$\delta_x \eta_{Mk} = \frac{h}{2a_0}\left(f_{Mk} - i\delta_{\bar{t}}\eta_{Mk} - v_M\phi_{Mk}\right), \ k = \overline{1,N}. \tag{62}$$

Using (59)-(62) we write iterations $[v]_m$ for the discrete problem (53)-(57) as follows:

$$[v]_m = P_{V_m}\{[v]_m - \beta I'_m([v]_m)\}, \tag{63}$$

where P_{Vm} is projection of the an element in the set V. Considering definition of the V we write projections as follows:

$$(v_j)_m = \begin{cases} (v_j)_m + \beta_n(I'_m([v]_m))_j, & b_0 \leq (v_j)m - \beta_m(I'_m([v]_m)_j \leq b_1 \\ b_{0,} & (v_j)_m - \beta_m(I'_m([v]_m)_j < b_0 \\ b_1, & (v_j)m - \beta_m(I'_m([v]_m)_j > b_1 \end{cases}$$

for $j = \overline{0,M}$, $m = 0,1,2,\ldots$. Now let us choose β_n and α^m. For the first step let be $m = 1$, $\alpha^1 = \alpha$, such that $\alpha > 1$ is a constant. Firstly, let us take $\beta_n = \beta$, $\beta > 0$ and check the condition

$$I_m([v]_{m+1}) \leq I_m([v]m). \tag{64}$$

If the contiditon (64) doesn't satisfy then we divide the number β, until (64) holds. In this case, if the condition

$$\left\{h\sum_{h=1}^{M-1}\left|(v_j)_{m+1} - (v_j)_m\right|^2 + \frac{h}{2}\left|(v_0)_m - (v_0)_m\right|^2 + \right. \tag{65}$$

$$\left.\frac{h}{2}\left|(v_M)_{m+1} - (v_M)_m\right|^2\right\}^{1/2} \leq \epsilon$$

satisfies then we can stop the iteration process, where $\epsilon > 0$ is a given number. Now, let us check the conditons

$$|I_m([v]_{m+1}) - \alpha^m \Bigg\{ h \sum_{h=1}^{M-1} \Big|(v_j)_{m+1} - (v_j)_m\Big|^2 + \frac{h}{2}\Big|(v_0)_m - (v_0)_m\Big|^2 + \qquad (66)$$

$$\frac{h}{2}\Big|(v_M)_{m+1} - (v_M)_m\Big|^2 \Bigg\}^{1/2} \leq \epsilon_1$$

for the $\alpha^m = \alpha$, where $\epsilon_1 > 0$ is a given number.

If contidition (66) doesn't satisy then we check condition (65) for $\alpha^m = \alpha\delta^{-m}$ again, where $\delta > 1$ is a constant. When the condition (66) holds, we stop iterations.

5. Applications to Test Problem

Now, in a quantum-mechanical problem, we will test this minimization algorithm. We will consider the state of a hormonic osilator with potential v. This harmonic osilator is in a field of force f. We examine the best appropiate potential v for which osilator has the maximum probability to be at given position y.

In the following examples, l and T are bondaries of the field. $y(x)$ is a given position and $f(x,t)$ is a field of force. Fortran-90 programs were written for these examples. The results of the programs are given in tables and graphs. The boundary conditions (3) were written as

$$\left.\frac{\partial\psi}{\partial x}\right|_{x=0} = g_0(t), \qquad \left.\frac{\partial\psi}{\partial x}\right|_{x=l} = g_1(t)$$

for the approximate solution of the problem (1)-(4)

Example 1 *Let us assume as* $l = 1,\ T = 1, a_0 = 1,\ f(x,t) = -ix(x+t),\ \varphi(x) = ix$ $g_0(t) = 0,\ g_1(t) = 0,\ y(x) = i(x+1),\ \alpha = 0.09$ *and* $N = 20$ *for the numerical solution of the problem (1)-(3), (6). In this case exact solution of the problem is* $v^*(x) = x$. *The exact solution and approximate solution are given in Table 1 and Figure 1.*

Table 1. $v^*(x_i)$ exact solution; $v(x)$ approximate solution.

x_i	$v^*(x_i)$	$v(x_i)$	$\lvert v^*(x_i) - v^*(x_i)\rvert$
.050	.0500000000	-.0307098000	.0807098000
.100	.1000000000	.0210873400	.0789126600
.150	.1500000000	.0728603500	.0771396500
.200	.2000000000	.1246068000	.0753932400
.250	.2500000000	.1763250000	.0736750200
.300	.3000000000	.2280143000	.0719857100
.350	.3500000000	.2796749000	.0703250500
.400	.4000000000	.3313079000	.0686920600
.450	.4500000000	.3829152000	.0670847900
.500	.5000000000	.4344996000	.0655004100
.550	.5500000000	.4860646000	.0639354000
.600	.6000000000	.5376147000	.0623853200
.650	.6500000000	.5891553000	.0608447800
.700	.7000000000	.6406924000	.0593076300
.750	.7500000000	.6922330000	.0577670300
.800	.8000000000	.7437849000	.0562151100
.850	.8500000000	.7953570000	.0546430300
.900	.9000000000	.8469588000	.0530412200
.950	.9500000000	.8986009000	.0513991100

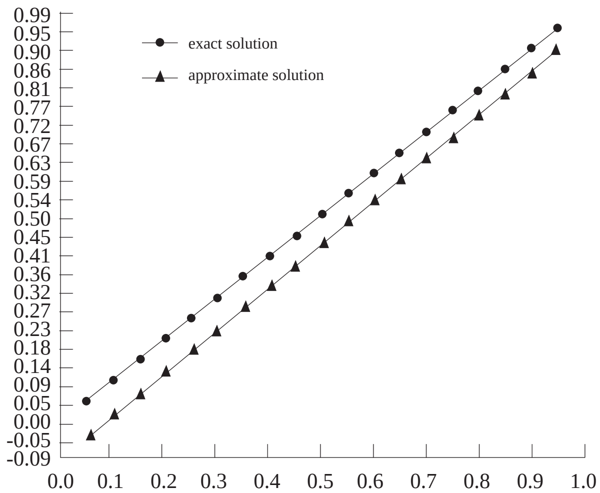

Figure 1. Graph of the $v^*(x) = x$ and approximate solution.

Example 2 *Let us assume as* $l = 1, T = 1, a_0 = 1, f(x,t) = 2i - i(x^2+t)\sin x - 1,\ \varphi(x) = ix,\ y(x) = i(x^2+1),\ \alpha = 0.09$ *and* $N = 20$ *for the numerical solution of the problem (1)-(3), (6). In this case exact solution of the problem is* $v^*(x) = \sin x$. *The exact solution and approximate solution are given in Figure* 2.

Table 2. $v^*(x_i)$ exact solution; $v(x)$ approximate solution.

x_i	$v^*(x_i)$	$v(x_i)$	$\lvert v^*(x_i) - v^*(x_i)\rvert$
.050	.0499791700	.1223487000	.0723695500
.100	.0998334200	.1607708000	.0609373400
.150	.1494381000	.1990807000	.0496425500
.200	.1986693000	.2371852000	.0385159000
.250	.2474040000	.2749923000	.0275882900
.300	.2955202000	.3124059000	.0168856400
.350	.3428978000	.3493373000	.0064395070
.400	.3894183000	.3856939000	.0037244260
.450	.4349656000	.4213871000	.0135784700
.500	.4794255000	.4563275000	.0230980800
.550	.5226873000	.4904303000	.0322569600
.600	.5646425000	.5236107000	.0410317800
.650	.6051864000	.5557873000	.0493991400
.700	.6442177000	.5868798000	.0573378200
.750	.6816388000	.6168110000	.0648277400
.800	.7173561000	.6455055000	.0718505400
.850	.7512804000	.6728895000	.0783909000
.900	.7833269000	.6988956000	.0844312900
.950	.8134155000	.7234555000	.0899599800

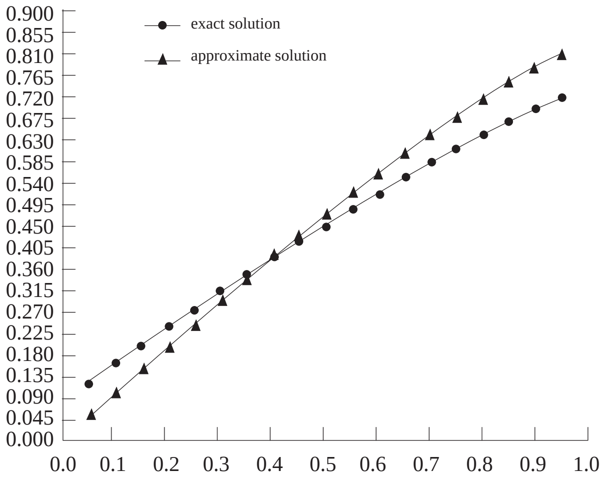

Figure 2. Graph of the $v^*(x) = \sin x$ and approximate solution.

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