FINITE DIFFERENCE METHOD
FOR AN OPTIMAL CONTROL PROBLEM
OF QUANTUM PROCESSES

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0. INTRODUCTION

In recent years there has been growing interest in general problems of control of objects governed by equations of quantum mechanics, electrodynamics and quantum fields. See [1] and [2 - 6] for an up-to-date survey and an extensive bibliography. A typical class of these problems is encountered in nuclear energetics, automatics and computer engineering techniques. Unfortunately, theoretical researches have been extensively developed, only few results have been published on approximate methods for these problems [7].

The aim of the present paper is to suggest a scheme based on the finite difference method for approximating a nonlinear optimal control problem of quantum processes governed by nonstationary Schrödinger equations.

In Section 1 we describe the optimal control problem to be studied. Then in Section 2 we develop the finite difference scheme for this problem. The main results are formulated in Section 3 and established in Section 4.

Throughout the paper we shall use the notations of [8].

1. OPTIMAL CONTROL PROBLEM OF QUANTUM PROCESSES

Let $\Omega$ be a bounded domain of $\mathbb{R}^n$, $T$ be a given finite, positive number, $Q = \Omega \times [0, T]$, $S = \Gamma \times [0, T]$, where $\Gamma$ is the boundary of $\Omega$. Consider the following system

$$\frac{\partial \Psi}{\partial t} - i \sum_{k, j=1}^{n} \frac{\partial}{\partial x_k} \left( a_{kj}(x) \frac{\partial \Psi}{\partial x_j} \right) + i a(x) \Psi + iu(x) \Psi = 0 \quad (1.1)$$

$$\Psi|_{\partial \Omega} = 0, \quad (x, t) \in Q \quad (1.2)$$
\[ \psi_{t=0} = \varphi(x), \ x \in \Omega, \]  
\[ \| \psi \| = 1, \| \cdot \| = \| \cdot \|_{L^2(\Omega)}, \]

where

(i) \( a_{kj}, a(x) \) belong to the real functional space \( L_\infty(\Omega) \),

(ii) \( u(x) \in L_\infty(\Omega), q = \begin{cases} n + \varepsilon & \forall \varepsilon > 0, n = 2 \\ n & n > 2 \end{cases} \)

(iii) \( a(x), u(x) \geq 0 \) almost everywhere in \( \Omega \),(iv) a_{kj}(x) = a_{jk}(x) \quad k, j \in [1, 2, \ldots, n], 

(vi) \| \partial a_{kj} \| / \partial x_j \leq \mu_3,

(vii) \( \Omega \) is a ball, or a ball layer, or a parallelepiped or \( \Omega \) can be transformed into one of these domains with the aid of a regular transformation \( y = y(x) \in C^2(\Omega) \). \( \mu_1, \mu_2, \mu_3 \) are fixed and positive constants, \( \xi = (\xi_1, \ldots, \xi_n) \) is an arbitrary vector of \( \mathbb{R}^n \), \( |\xi|^2 = \xi_1^2 + \ldots + \xi_n^2 \).

**Definition.** A function \( \psi \) is said to be a generalized solution in \( W^{1,1}_2(Q) \) of the problem (1.1) -- (1.3), if \( \psi \) belongs to \( W^{1,1}_2(Q) \) and satisfies

\[
\frac{\partial}{\partial t} \psi \eta + i \sum_{k,j=1}^{n} a_{kj} \psi x_k \overline{\eta} x_j + ia \psi \overline{\eta} dx dt \\
+ i \int_Q u \psi \overline{\eta} dx dt = \int_{\Omega} \overline{\psi}(x, 0) \overline{\eta} dx
\]

for all \( \eta \) from \( W^{1,1}_{2,0}(Q) \).

Further, let

\[ \varphi \in W^{2}_{2,0}(\Omega). \]

Then the problem (1.1) -- (1.3) has a unique generalized solution in \( W^{1,1}_2(Q) \) ([2]). Furthermore, this solution be belongs to \( W^{2,1}_2(Q) \). Consequently, \( \psi(x, T; u) \) makes sense and \( \psi(x, T; u) \in W^{2}_2(Q) \). From [2] we also have

\[ \| \psi(x, t; u) \| = \| \varphi \| = 1, \quad \forall \ t \in [0, T] \]

Let \( \varepsilon(x) \) be a given function from \( W^{2}_{2,0}(\Omega) \). Suppose that the control \( u(x) \) belongs to a bounded closed and convex subset \( \mathcal{U} \) of \( L^+_q(\Omega) \). \( L^+_q(\Omega) = \{ u(x) | u(x) \in L^q(\Omega), u(x) \geq 0 \text{ almost everywhere in } \Omega \} \). The control problem we are concerned with is to minimize the functional
\[ J(u) = \int_\Omega \| \psi(x, T; u) - z(x) \|^2 \, dx = \| \psi(x, T; u) - z(x) \|^2 \]  
subject to the above constraints.

This problem arises from the control of quantum processes ([1], [6]). It is known [6] that under the above mentioned conditions it always has a solution.

### 2. Finite Difference Scheme for the Problem

Let the upper-half space \( E_n \times [0, \infty) \) of variables \((x, t)\) be covered by a grid \( x_i = k_i h_i, h_i \geq 0, k_i \in \{0, \pm 1, \pm 2, \ldots\}, i \in \{1,2,\ldots, n\} \) and \( t = k_0 \tau, \geq 0, k_0 \in \{0,1,2,\ldots\} \). Let \( Q(k, k_0) = \omega(kh) \times (k_0 \tau, (k_0+1) \tau) = \{ (x, t) : k_i h_i \leq x_i \leq (k_i+1) h_i, k_0 \tau \leq t \leq (k_0+1) \tau \} \). By \( \overline{\Omega}_h \) we denote the closed domain consisting of these cells \( \omega(kh) \) which are contained in \( \overline{\Omega} \). Let \( S_h \) be the boundary of \( \overline{\Omega}_h \) and \( \Omega_h = \overline{\Omega}_h \setminus S_h \). For functions \( \psi \) defined on our grid we use the notation \( \psi_h \), but occasionally for the sake of simplicity we write \( \psi \) instead of \( \psi_h \) if no confusion is possible. Further, \( \psi_h(k) \) denotes the restriction of the grid function \( \psi_h \) to the layer \( t = t_k = k\tau \).

Let
\[
\sigma \psi_h(k) = \frac{1}{2} [\psi_h(k) + \psi_h(k+1)],
\]

\[
\mathbf{u}_h \bigg|_{\omega(kh)} = (\Delta h)^{-1} \mathbf{u}(x) dx, \quad \Delta h = h_1 h_2 \ldots h_n,
\]

\[
\mathbf{e}_h \bigg|_{x=kh, t=k_0 \tau} = (\Delta h)^{-1} \tau^{-1} \int_{(k_0-1) \tau}^{k_0 \tau} \int_{\omega(kh)} \xi(x,t) dxdt,
\]

where \( \xi(x,t) \) is any function from \( L_2(Q_T) \).

For any grid \( \Omega_h \) consider the following problem

\[
I_h, \tau ([u]_h) = (\Delta h)^2 \sum_{k} \| \psi_h(N) - z_h \|^2 \rightarrow \inf,
\]

\[
\psi_h(k+1) - \psi_h(k) \over \tau - i \sum_{l,j=1}^{n} (a_{lj} h \sigma \psi_h(k)) x_j \tau - i a_h \sigma \psi_h(k) + i u_h \sigma \psi_h(k) = 0,
\]

in \( \Omega_h, k \in \{0,1,2,\ldots, N\} = \left[ \frac{T}{\tau} \right] \),

\[
\psi_h(k) |_{S_h} = 0,
\]
\[ \psi_h(0) = \varphi_h \text{ in } \Omega_h, \quad (2.4) \]
\[ [u]_h \in U_h = \{ [u]_h = \{ u_h \}, u_h \in \mathcal{U} \}, \quad (2.5) \]

where \( \psi_h(k, [u]_h) \) is a solution of the problem (2.2)–(2.4) corresponding to control \([u]_h\).

We shall assume that for every grid \( \Omega_h \times \omega \) by any available minimization method one can compute the approximate value \( I_{h, \tau}^* \downarrow \varepsilon_{h, \tau} \) of the infimum \( I_{h, \tau}^* \) of the function \( I_{h, \tau} \) in \( U_h \) subject to conditions (2.2)–(2.5) and approximate control \([u]_{h, \varepsilon} = \{ u_h \}, u_h \in \mathcal{U} \) such that

\[ I_{h, \tau}^* \leq I_{h, \tau}([u]_{h, \varepsilon}) \leq I_{h, \tau}^* \downarrow \varepsilon_{h, \tau}, \quad (2.6) \]

where \( \varepsilon_{h, \tau} \) converges to zero as \( h \downarrow 0, \tau \downarrow 0 \) and \( h \) and \( \tau \) tend simultaneously to zero.

3. FORMULATION OF THE MAIN RESULTS

For every function \( \psi_{h, \tau}(k) \) defined on a grid \( \Omega_h \times \omega \) we put

\[ \tilde{\psi}_{h, \tau}(x,t) = \begin{cases} \psi_h(t), & (x,t) \in \omega_{(kh)} \times \omega \tau, \\
0, & (x,t) \in \omega_{(kh)} \times \omega \tau. \end{cases} \]

THEOREM 1. The finite difference scheme (2.2)–(2.4) has a unique grip solution \( \psi_{h, \tau} \) and its interpolation \( \tilde{\psi}_{h, \tau}(x,t) \) strongly converges in \( \bar{W}_{2,2}^1(Q) \) to the generalized solution in \( \bar{W}_{2,2}^1(Q) \) of the problem (1.1)–(1.3) \( \psi(x,t) \) as \( h \downarrow 0, \tau \downarrow 0 \). Furthermore

\[ \| \tilde{\psi}_{h, \tau} \| = \| \varphi_h \| \quad (2.7) \]

and

\[ \| \psi(x,t) \big|_{t=k} - \tilde{\psi}_{h, \tau}(x,t) \big|_{t=k} \|^2 \leq c(\tau + (\Delta h)^2), \quad (2.8) \]

where the constant \( c \) does not depend on \( \tau \) and \( h \), but depends only on the domain \( \Omega \) and the coefficients of equation (1.1).

THEOREM 2. Let \( u^* \) be a solution of the problem (1.8). Then

\[ \lim_{h \downarrow 0, \tau \downarrow 0} I^* = J^* = \inf_{u \in \mathcal{U}} J(u), \quad (h, \tau \downarrow 0) \]

\[ -c_1(\omega_{u^*}(h) + \sqrt{\tau + (\Delta h)^2}) \leq I^* - J^* \leq c_2 \sqrt{\tau + (\Delta h)^2}, \quad (2.9) \]
where $\omega_u(h)$ is the module of continuity of $u(x)$ in $L^q(\Omega)$. If the sequence
\[
\{[u]_{h,\varepsilon}\}
\]
determined from (2.6), then
\[
0 \leq J ([u]_{h,\varepsilon}) - J^* \leq c_3 (\omega_u(h) + \sqrt{\tau + h})^2 + \varepsilon_{h,\tau}
\]
(2.10)

4. PROOFS OF THE CONVERGENCE THEOREMS

Proof of Theorem 1. From (2.2) we have
\[
\psi_h (k + 1) - i \frac{\tau}{2} \sum_{h,j=1}^n (a_{ijh} \psi_j (k + 1)) x_{i_l} + i \frac{\tau}{2} (a + u_h) \psi_h (k + 1) =
\]
\[
= \psi_h (k) + i \frac{\tau}{2} \sum_{l,j=1}^n (a_{ijh} \psi_j (k)) x_{i_l} - i \frac{\tau}{2} (a + u_h) \psi_h (k)
\]
in $\Omega_h$, $k \in \{0, 1, \ldots, N - 1\}$.

Let $\psi(k) = \{ \psi_h (k) \}$, let $H_h$ be the linear space of all vector-functions defined in $\Omega_h$. From (4.1), (2.3), (2.4) we have
\[
(E - i \frac{\tau}{2} L_h) \psi (k + 1) = (E + i \frac{\tau}{2} L_h) \psi (k),
\]
where $E$ is the identity operator in $H_h$, $L_h$ is the operator defined by the system (4.1) and the condition (2.3).

Operator $L_h$ acts in the finite dimensional space $H_h$ so it is bounded. Further, conditions (1.7), (1.8) and (2.3) mean that $L_h$ is symmetric (or self-adjoint) and negative defined. Therefore, the spectrum of the operator $A$ is real. Consequently, the operator $E - i \frac{\tau}{2} L_h$ has an inverse bounded operator.

Now, by the above and (4.2) we obtain
\[
\psi (k + 1) = (E - i \frac{\tau}{2} L_h)^{-1} ((E + i \frac{\tau}{2} L_h) \psi (k).
\]

Operator $K = (E - i \frac{\tau}{2} L_h)^{-1} (E + i \frac{\tau}{2} L_h)$ is the Kelleg transform of the self-adjoint operator $L_h$, so it is isometric ([10], point 121). Therefore
\[
\| \psi (k + 1) \|_{H_h}^2 = (\Delta h)^2 \sum_{\Omega_h} | \psi_h (k + 1) |^2
\]
\[
= (\Delta h)^2 \sum_{\Omega_h} | \psi_h (k) |^2 = \| \psi (k) \|_{H_h}^2
\]
\( \| \tilde{\psi}_h (k+1) \| ^2 = \| \tilde{\psi}_h (k) \| ^2 \). From this equality, it is easy to see that

\[
\| \tilde{\psi}_h (k) \| ^2 = \tilde{\psi}_h \| ^2, \quad \forall k \in [1, 2, \ldots, N].
\]

The proof of the convergence of the finite difference scheme (2.2) - (2.4) is similar to the one in [8] and [9], and therefore will be omitted. Now, we study the accuracy of this scheme.

Let

\[
y_h (k) = \frac{1}{\Delta h} \int_{\omega (kh)} \psi (x, k\tau) \, dx,
\]

\[
z_h (k) = \psi_h (k) - y_h (k).
\]

We have

\[
\left( E - i \frac{\tau}{2} L_h \right) z(k+1) = \left( E + i \frac{\tau}{2} L_h \right) z(k)
\]

\[
= - \left( E - i \frac{\tau}{2} L_h \right) y(k+1) + \left( E + i \frac{\tau}{2} L_h \right) y(k).
\]

Hence,

\[
z (k+1) = Kz(k) - y(k) + Ky (z)
\]

and

\[
\| \tilde{z} (k+1) \| ^2 \leq \| \tilde{z} (k) \| ^2 + \| \tilde{y} (k+1) - y (k) \| ^2 + \| (E-K) y(k) \| ^2.
\]

On the other hand

\[
\| \tilde{y} (k+1) - \tilde{y} (k) \| ^2 \leq \| \psi (x, (k+1) \tau) - \psi (x, k\tau) \| ^2
\]

\[
= \tau^2 \left\| \frac{\partial \Psi (x, \theta)}{\partial t} \right\|^2 \leq \tau^2, \quad k\tau \leq \theta \leq (k+1)\tau.
\]

From conditions (i) - (vii) it is easy to see that \( \| E - K \| \leq \tau \).

Hence,

\[
\left\| \left( E - i \frac{\tau}{2} L_h \right)^{-1} L_h \right\|^2 \leq \tau.
\]

(Throughout the sequel \( c, c_1, c_2, \ldots \) denote a generic positive constant independent of \( h \) and \( \tau \)).

Finally, we have

\[
\| \tilde{z} (k+1) \| ^2 \leq \| \tilde{z} (k) \| ^2 + c\tau \leq \cdots \leq \| z(0) \| ^2 + k\tau \leq c\tau.
\]

Consequently,

\[
\| \Psi_h (k+1) - \Psi (x, (k+1) \tau) \| ^2 \leq \| \Psi_h (k+1) - \tilde{y}_h (k+1) \| ^2
\]

\[
+ \| \tilde{y}_h (k+1) - \Psi (x, (k+1) \tau) \| ^2 \leq c\tau + \| \tilde{y}_h (k+1) - \Psi (x, (k+1) \tau) \| ^2
\]

\[
\leq c\tau + \sum_{h} \Delta h \int_{\Omega_h} \Psi (x, (k+1) \tau) \, dx - \Psi (x, (k+1) \tau) \| ^2_{\omega (kh)}
\]
\[
\begin{aligned}
= c \tau + \sum \int \limits_{\Omega_h} \left( \Psi(x, (k + 1) \tau) - \Psi(x, (k + 1) \tau) \right) d\| \omega \|_{\Omega(h)}^2 \\
= c \tau + \sum \int \limits_{\Omega_h} \left( \int \left( \Psi(x, (k + 1) \tau) - \Psi(x, (k + 1) \tau) \right) d\| x \|_{\omega(kh)}^2 \\
= c \tau + \sum \int \limits_{\Omega_h} \left( \frac{1}{\Delta h} \int \Psi(x, (k + 1) \tau) d\| x \|_{\omega(kh)}^2 \\
= c \tau + \sum \int \limits_{\Omega_h} \left( \frac{1}{\Delta h} \int \Psi(x, (k + 1) \tau) d\| x \|_{\omega(kh)}^2 \\
\leq c \tau + \sum \int \left( \frac{1}{\Delta h} \int \frac{\partial \Psi}{\partial \eta} d\eta \right)^2 \\
= c \tau + \sum \int \left( \frac{1}{\Delta h} \int \frac{\partial \Psi}{\partial \eta} d\eta \right)^2 \\
\leq c \tau + (\Delta h)^2 \left( \frac{\partial \Psi}{\partial \eta} \right)^2 \\
\leq c \tau + (\Delta h)^2 \left( \frac{\partial \Psi}{\partial \eta} \right)^2. \\
\end{aligned}
\]

Thus,

\[
\| \tilde{\Psi}_h(k + 1) - \Psi(x, (k + 1) \tau) \| \leq c(\tau + (\Delta h)^2).
\]

Theorem 1 is proved.

**Proof of Theorem 2.** We shall need some lemmas.

**Lemma 1.** (F.P. Vasilyev [11], p. 299). Let \( U \) be a convex, closed set of \( L_\infty(\Omega) \), \( u(x) \) an element of \( U \). Then

\[
u \in U \quad \text{(4.3)}
\]

**Lemma 2.** Let all the conditions of Theorem 1 hold. Then for every \( u \in U \) we have

\[
| J(u) - I_{h, \tau}(\lceil u \rceil) | \leq c \sqrt{\tau + (\Delta h)^2}.
\]

**Proof.** From Lemma 4.1 [8] (p. 301) we have

\[
| z(x) - z(x) | \to 0 \text{ as } h \to 0.
\]

Further, since \( z(x) \in W_{2,0}^2(\Omega) \) it follows that

\[
| z(x) - z(x) | \leq c(\Delta h)^2 \left( \frac{\partial z}{\partial x} \right)^2.
\]

On the other hand

\[
I_{h, \tau}(\lceil u \rceil) = (\Delta h)^2 \sum \int \frac{\Psi_{h, \tau}(N_\Omega \lceil u \rceil - z_h)}{h}^2
\]

\[
= \| \tilde{\Psi}_{h, \tau}(x, T; u) - \tilde{z}(x) \|^2.
\]
\[
\left| J(u) - I_{h, \tau}([u]_h) \right| = \left| \| \Psi(x,T; u) - z(x) \| ^2 \\
- \left\| \hat{\Psi}_{h, \tau}(x,T; u) - \hat{z}(x) \right\| ^2 \right|
\leq \left( \| \Psi(x,T; u) \| + \| \hat{\Psi}_{h, \tau}(x,T; u) \| + \| z(x) \| + \| \hat{z}(x) \| \right) \times
\left( \| \Psi(x,T; u) - \hat{\Psi}_{h, \tau}(x,T; u) \| + \| z(x) - \hat{z}(x) \| \right).
\]

From (1.7), (4.5) and (2.8) we get
\[
\left| J(u) - I_{h, \tau}([u]_h) \right| \leq c \sqrt{\tau + (\Delta h)^2}.
\]

**Lemma 2.** Let all the conditions of Theorem 1 hold and [u] be any control from $U$. Then
\[
\left| J([\tilde{u}]_h) - I_{h, \tau}([u]_h) \right| \leq c(\omega_u(h) + \sqrt{\tau + (\Delta h)^2}),
\]
where $\omega_u(h)$ is the module of continuity of $u(x)$ in $L_2(\Omega)$.

**Proof.** Using the inequality for the coefficients of the equation (1.1) ([2] and 6), p. 18) we can write
\[
\left| J([\tilde{u}]_h) - I_{h, \tau}([u]_h) \right| \leq c \left( \| \Psi(x,T; [\tilde{u}]_h) \\
- \tilde{\Psi}_{h, \tau}(x,T; [u]_h) \| + \| z(x) - \hat{z}(x) \| \right)
\leq c \left( \| \Psi(x,T; [\tilde{u}]_h) - \Psi(x,T; u) \| + \| \Psi(x,T; u) - \\
- \tilde{\Psi}_{h, \tau}(x,T; [u]_h) \| + \| z(x) - \hat{z}(x) \| \right)
\leq c \left( \| [\tilde{u}]_h - u \| _q + \sqrt{\tau + (\Delta h)^2} + \Delta h \right)
\leq c(\omega_u(h) + \sqrt{\tau + (\Delta h)^2}).
\]

Let us now prove Theorem 2. As seen above, the set of all optimal controls of the problem (1.8) $U_*$ is non-empty. Let us pick $u^* \in U_*$. According to Lemma 1 $[u^*_h]_h \in U$. Consequently, it follows from Lemma 2 that
\[
I_{h, \tau}^* \leq I_{h, \tau}([u^*_h]_h) \leq J(u^*) + c \sqrt{\tau + (\Delta h)^2}
= J^* + c \sqrt{\tau + (\Delta h)^2}.
\]

Further, the function $I_{h, \tau}([u]_h)$ attains its infimum on the compact set $U_h$, i.e., $I_{h, \tau} \rightarrow -\infty$, $U_\tau \neq \emptyset$. Since $U$ is convex we have $[u^*_h]_h \in U$. Now, from Lemma 3 we get
\[
J^* \leq J([u^*_h]_h) < I_{h, \tau}([u^*_h]_h) + c(\omega_u(h) + \\
+ \sqrt{\tau + (\Delta h)^2}) = I_{h, \tau}^* + c(\omega_u(h) + \sqrt{\tau + (\Delta h)^2}).
\]
Hence,
\[ -c(\omega_u, (h) + \sqrt{\tau + (\Delta h)^2}) \leq I^*_{h, \tau} - J^* \leq c \sqrt{\tau + (\Delta h)^2}. \]

Since \( \omega_u(h) \to 0 \) as \( h \to 0 \) ([12], §3), we get
\[ \lim_{(h, \tau) \to 0} I^*_{h, \tau} = J^*. \]

Consider a sequence \( \{[u]_{h, \tau}\} \) determined by \( (2.6) \). Clearly,
\[ [u]_{h, \tau} \in U \text{ and} \]
\[ 0 \leq J([u]_{h, \tau}) - J^* = \left[ J([u]_{h, \tau}) - J^*([u]_{h, \tau}) \right] + \left[ I^*_{h, \tau} - J^* \right]. \]

From \( (2.6), (4.4), (4.6) \) we then obtain
\[ J([u]_{h, \tau}) - J^* \leq c(\omega_u(h) + \sqrt{\tau + (\Delta h)^2}) + \varepsilon_{h, \tau}. \]

This means that the sequence \( \{[u]_{h, \tau}\} \) is a minimizing sequence for the problem \( (1.8) \).

The proof of Theorem 2 is complete.

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