

### Abstract

In the class of nonlinear optimal control problems, optimality conditions are constructed in the form of fixed point problems for certain control operators. The fixed point problems under consideration make it possible to obtain necessary conditions for the optimality of a control that are stronger than the maximum principle and to construct new iterative methods for finding extremal controls that satisfy the optimality conditions. The proposed methods, in contrast to the known gradient methods, are characterized by the possibility of rigorous improvement of non-optimal controls that satisfy the maximum principle. The constructed methods can find degenerate extremal controls for which the maximum principle degenerates. These properties of the proposed fixed point methods and their computational efficiency in comparison with known methods are illustrated by model examples.

### Introduction

Mathematical formulations of topical problems of optimal control of quantum systems have been considered in the works of many researchers [1]. In the works of V.F. Krotov, V.I. Gurman, and of their followers [2,3] there are studied classes of controlled quantum systems described by ordinary differential controls linear in state and control with nonlinear optimality criteria.

Features of the selected class of problems are indicated. First, it is the high dimension of the system state vector. The second feature is the absence of restrictions on the state, including terminal restrictions. The third feature is the use of a scalar control function characterizing the electric field. In this class, the search for an optimal solution based on standard necessary optimality conditions in the form of a boundary value problem of the maximum principle causes significant difficulties due to the large dimension. To find solutions, iterative methods for improving control are usually used. In particular, the global Krotov method was used as a tool for finding solutions to problems, which was compared in efficiency with the known gradient method [4].

In this paper, iterative methods for finding controls that satisfy the maximum principle are proposed based on the construction of operator problems about a fixed point in the space of controls, which are equivalent to the boundary value problem of the maximum principle. This approach for representing optimality conditions for control is modified and studied in the considered class of optimization problems for quantum control systems, which is characterized property of singularity of extremal solutions.

### Methods

A model class of optimal control problems for quantum systems with a quadratic optimality criterion is considered:

$$\dot{x}(t) = (A + u(t)B)x(t), \quad x(t_0) = x^0, \quad u(t) \in U \subset \mathbb{R}, \quad t \in T = [t_0, t_1],$$

$$\Phi(u) = \langle x(t_1), Lx(t_1) \rangle \rightarrow \inf_{u \in U},$$

where  $x(t) = (x_1(t), \dots, x_n(t))$  is the state vector of the system,  $L$  is a real symmetric matrix,  $A$  and  $B$  are real matrices. As admissible controls  $u(t)$ ,  $t \in T$ , a set  $V$  of piecewise continuous scalar functions on an interval  $T$  with values in a compact and convex set  $U \subset \mathbb{R}$ . The initial state  $x^0$  and the interval  $T$  are fixed.

The Pontryagin function with a conjugate variable  $\psi$  and the standard conjugate system have the form:

$$H(\psi, x, u, t) = \langle \psi, (A + uB)x \rangle, \quad \psi \in \mathbb{R}^n,$$

$$\dot{\psi}(t) = -(A^T + u(t)B^T)\psi(t), \quad t \in T, \quad \psi(t_1) = -2Lx(t_1).$$

Let  $v \in V$ . We introduce possible notation:

$$x(t, v), \quad t \in T \text{ is the solution of the phase system}$$

$$\psi(t, v), \quad t \in T \text{ is the solution of the conjugate system}$$

Maximum principle for control  $u \in V$ :

$$u(t) = \arg \max_{u \in U} \langle \psi(t, u), Bx(t, u) \rangle, \quad t \in T.$$

$$u(t) = u^*(\psi(t, u), x(t, u)), \quad t \in T.$$

Let's define the mappings  $X, \Psi, V^*$  by the relations:

$$X(u) = x, \quad x(t) = x(t, u), \quad t \in T,$$

$$\Psi(u) = \psi, \quad \psi(t) = \psi(t, u), \quad t \in T,$$

$$V^*(\psi, x) = v^*, \quad \psi \in C(T), \quad x \in C(T), \quad v^*(t) = u^*(\psi(t), x(t)), \quad t \in T,$$

here  $C(T)$  the space of continuous functions on the interval  $T$ .

The maximum principle can be represented as an operator equation in the form of a fixed point problem in the control space with various constructable control operators  $G_1^*, G_2^*, G_3^*$ :

$$u = V^*(\Psi(u), X(u)) = G_1^*(u),$$

$$u = V^*(\Psi(u), X^*(\Psi(u))) = G_2^*(u),$$

$$u = V^*(\Psi^*(X(u)), X(u)) = G_3^*(u).$$

### Methods

On the set of admissible controls, each operator equation from relations is considered as a fixed point problem and has the following general form:

$$v = G(v), \quad v \in V.$$

To solve problem, an iterative process with index  $k \geq 0$  is proposed:

$$v^{k+1} = G(v^k), \quad v^0 \in V.$$

The calculations performed within the framework of the model problem [4] show a high quantitative and qualitative efficiency proposed methods of the maximum principle, which makes it possible to accurately calculate complex singular sections of extreme controls, which are typical in optimal control problems for quantum systems of the class under consideration.

### Conclusions

In the considered model class of controlled quantum systems, new operator forms of the maximum principle are constructed in the form of fixed point problems in the control space. With the help of the obtained new operator forms, new iterative algorithms are constructed based on the well-known apparatus of methods and the theory of fixed points, which make it possible to find extreme controls. In the developed iterative operator methods of searching for extreme controls, the following properties can be distinguished:

1. non-locality of successive control approximations;
2. computational stability, which standard methods for solving the boundary value problem of the maximum principle do not possess;
3. the absence of a time-consuming procedure for needle or convex control variation in a small neighborhood of the approximation under consideration, characteristic of gradient methods;
4. Numerical solution of Cauchy problems without constructing special auxiliary Krotov switching functions at each iteration of the constructed methods, in contrast to the well-known global Krotov method.

The above-mentioned properties of the proposed methods for finding extreme controls increase the efficiency of numerical solution of model problems in the class of quantum systems under consideration.

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