

Implicit Lyapunov Control of Multi-Control Hamiltonians Systems Based On the State Error

Fangfang Meng and Shuang Cong

Abstract—In the closed quantum system, if the control system is strongly regular and all other eigenstates are directly coupled to the target state, the control system can be asymptotically stabilized at the target eigenstate by the Lyapunov control based on the state error. However, if the control system is not strongly regular or as long as there is one eigenstate not directly coupled to the target state, the situations will become complicated. In this paper, we propose an implicit Lyapunov control method based on the state error to solve the convergence problems for these two degenerate cases. And at the same time, we expand the target state from the eigenstate to the arbitrary pure state. Especially, the proposed method is also applicable in the control system with multi-control Hamiltonians. On this basis, the convergence of the control systems is analyzed using the LaSalle invariance principle. Furthermore, the relation between the implicit Lyapunov functions of the state distance and the state error is investigated. Finally, numerical simulations are carried out to verify the effectiveness of the proposed implicit Lyapunov control method. The comparisons of the control effect using the implicit Lyapunov control method based on the state distance with that of the state error are given.

Keywords—Implicit Lyapunov control, state error, degenerate cases, convergence.

I. INTRODUCTION

IN the last 30 years, the control theory of quantum systems have developed rapidly, and it has been widely used in quantum chemistry, nanotechnology, quantum information, and quantum physics. Up to now, there have been many quantum methods, such as quantum optimal control, adiabatic control, the Lyapunov-based control, Optimal Lyapunov-based quantum control. The design idea of the Lyapunov-based control is based on the Lyapunov stability theorem, i.e., the control laws are designed by means of ensuring the first order time derivative of a selected Lyapunov function not to be positive. The control system based on the Lyapunov stability theorem is at least stable. However, the probability control in the quantum system requires a convergent control strategy, because a stable quantum control method may result in that the control system cannot reach the desired target state. Therefore in order to make the control system converge to the target state, it is necessary to study the convergence of the control system,

which is one of research focus of the Lyapunov-based control method.

Existing research results have indicated that: for the Schrödinger equation, in the case that the target state is an eigenstate, by using the Lyapunov control method based on the state distance [1] or the state error [2], [3], the control system can be asymptotically stabilized if two conditions are satisfied: i) The control system is strongly regular; ii) All other eigenstates, which are different from the target state, are directly coupled to the target state. The condition i) means that all differences of two energy levels are not mutually equal, i.e. the spectrum of the internal Hamiltonian is non-degenerate. And by using the Lyapunov method based on the average value of an imaginary mechanical quantity, two conditions which make the control system asymptotically stable are: i) The control system is strongly regular; ii) Every eigenstate of the internal Hamiltonian H_0 is directly coupled to other eigenstates [1], [4]. If the control system satisfies these two convergence conditions, it is called a non-degenerate case. Actually, many actual systems do not satisfy these conditions. These cases are called degenerate cases. In order to solve the convergence problems of the degenerate cases, several researchers introduced an implicit function to make the single control Hamiltonian quantum system converge to an eigenstate from any pure state [5]-[7]. In the multi-control Hamiltonians system, for the case that the target state is an eigenstate, by introducing a series of perturbations which are implicit functions and choosing an implicit Lyapunov function based on the state distance [8].

So far, for the Schrödinger equation, in the degenerate cases, the existing Lyapunov control methods can only make the control system converge to an eigenstate from any pure state. In the case that the target state is a superposition state, the convergence problem of the control system has not been resolved.

The main purposes of this paper are two points, the first is: For the Schrödinger equation, in the degenerate cases and the case that the target state is an arbitrary pure state, by using an implicit Lyapunov quantum control method based on the state error, we'll solve the convergence problem of the multi-control Hamiltonians system. Thus in the degenerate cases, the control system can completely transfer between two arbitrary pure states. Our basic idea is as follows: in order to solve the convergence problem of the degenerate cases for the multi-control Hamiltonians system, we introduce a series of implicit function perturbations and select a state error-based Lyapunov function which is an implicit function, too. This

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method is not a simple extension from the single control Hamiltonian case [7] to the multi-control Hamiltonians case. For the multi-control Hamiltonians case, the derivation process of the control laws and the convergence proof will become more complex, especially in the calculation of the first order time derivative of the Lyapunov function. On the other hand, to make the control system can also converge to a superposition state, we introduce a series of constant disturbances. The second contribution of this paper is to analyze the relationship between the implicit Lyapunov functions based on the state distance and the state error, and compare the control effects of these two implicit Lyapunov control methods.

The remainder of this paper is arranged as follows: In Section II, a convergent implicit Lyapunov control method based on the state error for the multi-control Hamiltonians system, and the convergence theorem of the control system are proposed, respectively. In Section III, the convergence theorem is proved by the LaSalle invariance principle. In Section IV, the relation between the implicit Lyapunov functions of the state distance and the state error is analyzed. In Section V, some numerical simulations are investigated. Some concluding remarks are drawn in Section VI.

II. CONTROL DESIGN

A N -level closed quantum system with multi-control Hamiltonians can be modeled as the following bilinear Schrödinger equation:

$$i|\dot{\psi}(t)\rangle = (H_0 + \sum_{k=1}^r H_k u_k(t) + \omega I)|\psi(t)\rangle \quad (1)$$

where $|\psi(t)\rangle$ is the state vector, H_0 is the internal Hamiltonian, $H_k, (k=1, \dots, r)$ are the control Hamiltonians, and $u_k(t)$ are scalar and real control laws, ω is the global phase control law.

For the Schrodinger equation, in the degenerate cases, the existing Lyapunov control methods can only make the control system converge to an eigenstate from any pure state. In order to making the control system can also converge to the target superposition state $|\psi_f\rangle$, we introduce a series of constant disturbances η_k . The dynamical equation (1) will become

$$i|\dot{\psi}(t)\rangle = (H_0 + \sum_{k=1}^r H_k (v_k(t) + \eta_k) + \omega I)|\psi(t)\rangle \quad (2)$$

where $v_k(t)$ and η_k are the control laws which need to design.

Our basic idea is: we add η_k to make the target state $|\psi_f\rangle$ is an eigenstate of $H_0 + \sum_{k=1}^r H_k \eta_k$, i.e.,

$$(H_0 + \sum_{k=1}^r H_k \eta_k)|\psi_f\rangle = \lambda'_f |\psi_f\rangle \quad (3)$$

where λ'_f is the eigenvalue of $H'_0 = H_0 + \sum_{k=1}^r H_k \eta_k$

corresponding to the target state $|\psi_f\rangle$. We can view H'_0 as the new internal Hamiltonian of the control system.

In the degenerate cases, in order to solve the convergence problem of the control system, we introduce perturbations $\gamma_k(t)$ which are implicit functions in the control laws $u_k(t), (k=1, \dots, r)$ of (1). The dynamical equation (2) will become

$$i|\dot{\psi}(t)\rangle = (H_0 + \sum_{k=1}^r H_k (\gamma_k(t) + v_k(t) + \eta_k) + \omega I)|\psi(t)\rangle \quad (4)$$

where $\gamma_k(t) + v_k(t) + \eta_k = u_k$ and ω are the total control laws.

The basic idea is as follows: Denote the system with the internal Hamiltonian H_0 , the control Hamiltonians $H_k, (k=1, \dots, r)$, and the control laws $\gamma_k(t) + v_k(t) + \eta_k = u_k$ as system 1, the system with the internal Hamiltonian

$H'_0 = H_0 + \sum_{k=1}^r H_k \eta_k$, the control Hamiltonians

$H_k, (k=1, \dots, r)$, and the control laws $\gamma_k(t) + v_k(t)$ as system 2, and the system with the internal Hamiltonian

$H_{03} = H_0 + \sum_{k=1}^r H_k (\gamma_k(t) + \eta_k)$, the control Hamiltonians

$H_k, (k=1, \dots, r)$, and the control laws $v_k(t)$ as system 3. All

these three systems can be depicted by (4). Denote the eigenvalues and eigenstates of H'_0 as $\lambda'_1, \lambda'_2, \dots, \lambda'_N$ and

$|\phi'_1\rangle, |\phi'_2\rangle, \dots, |\phi'_N\rangle$, respectively. Denote the eigenvalues and eigenstates of H_{03} as $\lambda'_{1, \gamma_1, \dots, \gamma_r}, \dots, \lambda'_{N, \gamma_1, \dots, \gamma_r}$ and

$|\phi'_{1, \gamma_1, \dots, \gamma_r}\rangle, \dots, |\phi'_{N, \gamma_1, \dots, \gamma_r}\rangle$, respectively, which are functions of the perturbations $\gamma_k(t)$. Without loss of generality, assume

$|\psi_f\rangle = |\phi'_g\rangle, 1 \leq g \leq N$. Denote $|\psi'_{f, \gamma_1, \dots, \gamma_r}\rangle = |\phi'_{g, \gamma_1, \dots, \gamma_r}\rangle$. If

one can design the perturbations $\gamma_k(t)$ such that i) $\omega'_{l, m, \gamma_1, \dots, \gamma_r} \neq \omega'_{i, j, \gamma_1, \dots, \gamma_r}, (l, m) \neq (i, j), i, j, l, m \in \{1, 2, \dots, N\}$,

where $\omega'_{l, m, \gamma_1, \dots, \gamma_r} = \lambda'_{l, \gamma_1, \dots, \gamma_r} - \lambda'_{m, \gamma_1, \dots, \gamma_r}$ holds; ii) For any

$|\phi'_{i, \gamma_1, \dots, \gamma_r}\rangle \neq |\psi'_{f, \gamma_1, \dots, \gamma_r}\rangle, (i=1, 2, \dots, N)$, there exists at least a $k \in \{1, \dots, r\}$ satisfying

$\langle \phi'_{i, \gamma_1, \dots, \gamma_r} | H_k | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle \neq 0, (k=1, \dots, r)$, and select the specific Lyapunov function based on the state error as

$$V(|\psi\rangle) = \frac{1}{2} \langle \psi - \psi'_{f, \gamma_1, \dots, \gamma_r} | \psi - \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle \quad (5)$$

then system 3 will converge to $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$. When system 3 converge to $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$, if the perturbations $\gamma_k(t)$ at $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$ are designed to equal zero, then system 3 will become system 2, and $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$ will become $|\psi_f\rangle$. Because the convergence of system 2 to $|\psi_f\rangle$ is equivalent to that of system 1 to $|\psi_f\rangle$, the convergence of system 1 to $|\psi_f\rangle$ will be ensured. In fact, the evolution of system 1 can be viewed as a composite of two evolution processes. One is system 3 converge to $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$ from the initial state $|\psi_0\rangle$, another one is $\gamma_k(t)$ converge to 0. In order to make the introduced perturbations take effect to make system 1 in the non-degenerate case converge to $|\psi_f\rangle$, the speed of $\gamma_k(t), (k=1,\dots,r)$ converging to 0 must be slower than the speed at which system 3 converges toward $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$. For convenience, the control system in the following Sections means system 1.

From the above analyses, we can design $\gamma_k(t)$ to be a monotonically increasing function on $V(t)$ as

$$\begin{aligned} \gamma_k(|\psi\rangle) &= \theta_k(V(|\psi\rangle)) \\ &= \theta_k\left(\frac{1}{2}\langle\psi - \psi'_{f,\gamma_1,\dots,\gamma_r} | \psi - \psi'_{f,\gamma_1,\dots,\gamma_r}\rangle\right), (k=1,\dots,r) \end{aligned} \quad (6)$$

where functions $\theta_k(\cdot)$ satisfy $\theta_k(0) = 0, \theta_k(s) > 0, \theta'_k(s) > 0$ for every $s > 0$, s is the independent variable of the function $\theta_k(\cdot)$. From (5) and (6), one can see that when we introduce implicit functions perturbations in the control laws to solve the convergence problems of the degenerate cases, accordingly, the selected Lyapunov function should be a implicit function of the time t . The existence of these implicit functions perturbations $\gamma_k(|\psi\rangle)$ in (6) can be depicted by lemma 1.

Lemma 1. Let $\theta_k \in C^\infty(R^+; [0, \gamma_k^*]), k=1,\dots,r, \gamma_k^* > 0$ satisfy $\theta_k(0) = 0, \theta_k(s) > 0, \theta'_k(s) > 0$ for every $s > 0, \|\theta'_k\|_\infty < 1/rC^*$, and $C^* = 1 + C$, $C = \max\left\{\left\|\left(\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k}\right)_{(\gamma_{10},\dots,\gamma_{r0})}\right\|_\infty; \gamma_{k0} \in [0, \gamma_k^*]\right\}$, $\gamma_{k0} = \gamma_k(0)$. Then for every state $|\psi\rangle \in S^{2N-1} = \{x \in C^N; \|x\|=1\}$, there exists a unique $\gamma_1, \gamma_2, \dots,$ and γ_r with $\gamma_k \in C^\infty(\gamma_k \in [0, \gamma_k^*]), (k=1,\dots,r)$ satisfying $\gamma_k(|\psi\rangle) = \theta_k\left(\frac{1}{2}\langle\psi - \psi'_{f,\gamma_1,\dots,\gamma_r} | \psi - \psi'_{f,\gamma_1,\dots,\gamma_r}\rangle\right)$ where R^+ represents the positive real number domain.

Proof:

Assume $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$ are analytic functions of $\gamma_k(|\psi\rangle) \in [0, \gamma_k^*]$, $\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k}$ is bounded on $[0, \gamma_k^*]$, thus $C < \infty$. The derivative of θ_k on γ_k is

$$\begin{aligned} \partial\theta_k\left(\frac{1}{2}\langle\psi - \psi'_{f,\gamma_1,\dots,\gamma_r} | \psi - \psi'_{f,\gamma_1,\dots,\gamma_r}\rangle\right) / \partial\gamma_k \\ = -\theta'_k \Re\left(\left\langle\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k} \middle| \psi\right\rangle\right). \end{aligned} \quad (7)$$

Let us define

$$F_k(\gamma_1, \dots, \gamma_r, |\psi\rangle) = \gamma_k - \theta_k\left(\frac{1}{2}\langle\psi - \psi'_{f,\gamma_1,\dots,\gamma_r} | \psi - \psi'_{f,\gamma_1,\dots,\gamma_r}\rangle\right),$$

where $F_k(\gamma_1, \dots, \gamma_r, |\psi\rangle)$ are regular.

For a fixed $|\psi\rangle \in S^{2N-1} = \{x \in C^N; \|x\|=1\}$, we have $F_k(\gamma_1(|\psi\rangle), \dots, \gamma_r(|\psi\rangle), |\psi\rangle) = 0, (k=1, \dots, r)$. Some deduction shows that

$$\frac{\partial F_k}{\partial\gamma_k(|\psi\rangle)} = 1 + \theta'_k \Re\left(\left\langle\psi \middle| \frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k} \right\rangle \langle\psi'_{f,\gamma_1,\dots,\gamma_r} | \psi\rangle\right) \quad (8)$$

where

$$\left|\Re\left(\left\langle\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k} \middle| \psi\right\rangle\right)\right| \leq \left|\left\langle\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k} \middle| \psi\right\rangle\right| \leq \left\|\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k}\right\|.$$

According to the given condition, we have

$$\left|\theta'_k \Re\left(\left\langle\frac{\partial|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle}{\partial\gamma_k} \middle| \psi\right\rangle\right)\right| < 1, \quad (9)$$

Then

$$\frac{\partial}{\partial\gamma_k(|\psi\rangle)} F_k(\gamma_1(|\psi\rangle), \dots, \gamma_r(|\psi\rangle), |\psi\rangle) \neq 0. \quad (10)$$

According to the implicit theorem [9], Lemma 1 is proved.

Next, on the basis of the Lyapunov stability theorem, let us design the control laws $v_k(t)$ and ω . The basic idea is that we design control laws to make the time derivative of the selected Lyapunov function be less than or equal to 0, i.e., $\dot{V}(t) \leq 0$.

Denote the eigenvalue of $H_{03} = H_0 + \sum_{k=1}^r H_k(\gamma_k(t) + \eta_k)$ correspond to $|\psi'_{f,\gamma_1,\dots,\gamma_r}\rangle$ as $\lambda'_{f,\gamma_1,\dots,\gamma_r}$. By (4) and (5), the time derivative of the selected Lyapunov function defined by (5) is

$$\dot{V} = -\sum_{k=1}^r \Re(\langle \langle \partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_k | \psi \rangle \rangle) \dot{\gamma}_k(t) - (\lambda'_{f, \gamma_1, \dots, \gamma_r} + \omega) \cdot \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | \psi \rangle \rangle) - \sum_{k=1}^r \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | H_k | \psi \rangle \rangle) v_k(t). \quad (11)$$

Equation (11) contains the time derivative of the implicit function perturbation $\dot{\gamma}$, which needs to be eliminated. For the multi-control Hamiltonians system, the elimination of $\dot{\gamma}$ will become more complicated than the single control Hamiltonian system proposed in [5]-[7]. By (6), one can deduce

$$\dot{\gamma}_j(t) = -\theta'_j \left(\sum_{k=1}^r \Re(\langle \langle \partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_k | \psi \rangle \rangle) \dot{\gamma}_k(t) + (\lambda'_{f, \gamma_1, \dots, \gamma_r} + \omega) \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | \psi \rangle \rangle) + \sum_{k=1}^r \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | H_k | \psi \rangle \rangle) v_k(t) \right) \quad (12)$$

Sum each item in both sides of (12), one has

$$\sum_{j=1}^r \dot{\gamma}_j(t) = -\sum_{j=1}^r \theta'_j \left(\sum_{k=1}^r \Re(\langle \langle \partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_k | \psi \rangle \rangle) \dot{\gamma}_k(t) + (\lambda'_{f, \gamma_1, \dots, \gamma_r} + \omega) \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | \psi \rangle \rangle) + \sum_{k=1}^r \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | H_k | \psi \rangle \rangle) v_k(t) \right) \quad (13)$$

Assume $\partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_1 = \dots = \partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_r$, and by (12), (13) becomes

$$\dot{V} = -\left[1 / (1 + \Re(\langle \langle \partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_k | \psi \rangle \rangle)) \sum_{j=1}^r \theta'_j \right] \cdot ((\lambda'_{f, \gamma_1, \dots, \gamma_r} + \omega) \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | \psi \rangle \rangle) + \sum_{k=1}^r \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | H_k | \psi \rangle \rangle) v_k(t)). \quad (14)$$

By the condition $\|\theta'_j\| < 1/(rC^*)$ in Lemma 1,

$(1 + \Re(\langle \langle \partial | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle / \partial \gamma_k | \psi \rangle \rangle)) \sum_{j=1}^r \theta'_j > 0$ holds. In order to ensure $\dot{V} \leq 0$, let us design ω and $v_k(t)$ as:

$$\omega = -\lambda'_{f, \gamma_1, \dots, \gamma_r} + cf_0 (\Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | \psi \rangle \rangle)), \quad (15)$$

$$v_k(t) = K_k f_k (\Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | H_k | \psi \rangle \rangle)), (k = 1, \dots, r), \quad (16)$$

where $K_k > 0$, $c > 0$ and $y_k = f_k(x_k), (k = 0, 1, \dots, r)$ are monotonic increasing functions through the coordinate origin of the plane $x_k - y_k$.

Equations (15) and (16) are the designed control laws by

using the Lyapunov stability theorem for the control system (4) with the Lyapunov function (5).

In fact, the above designed control laws can only ensure that the control system (4) is stable. In order to make the control system converge to the target state, we must analyze the convergence of the control system. Next, let us study the convergence of the control system. The results are described by Theorem 1.

Theorem 1: Consider the control system (11) with control fields $\gamma_k(t)$ designed in Lemma 1, η_k defined by (3), $v_k(t)$ designed in (17) and ω designed in (16). If the control system satisfies

- i) $\omega'_{l, m, \gamma_1, \dots, \gamma_r} \neq \omega'_{i, j, \gamma_1, \dots, \gamma_r}, (l, m) \neq (i, j), i, j, l, m \in \{1, 2, \dots, N\}$,
- where $\omega'_{l, m, \gamma_1, \dots, \gamma_r} = \lambda'_{l, \gamma_1, \dots, \gamma_r} - \lambda'_{m, \gamma_1, \dots, \gamma_r}$ holds; ii) For any $\langle \phi'_{i, \gamma_1, \dots, \gamma_r} \rangle \neq \langle \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle, (i = 1, 2, \dots, N)$, there exists at least a $k \in \{1, \dots, r\}$ satisfying

$\langle \phi'_{i, \gamma_1, \dots, \gamma_r} | H_k | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle \neq 0, (k = 1, \dots, r)$, then any state trajectory of the control system will converge toward $S^{2N-1} \cap E, E = \{ | \psi \rangle = e^{i\theta} | \psi_f \rangle, \theta \in R \}$.

This convergence theorem will be proved in Section III.

III. CONVERGENCE PROOF

According to the LaSalle invariance principle, as $t \rightarrow \infty$, any state trajectory will converge to the largest invariant set contained in the set E in which the states satisfy $\dot{V} = 0$.

The basic idea of the proof of Theorem 1 is: at first, the state set satisfying $\dot{V} = 0$ at some specific evolving moment is characterized. Then, whether $\dot{V} = 0$ holds after that moment is considered. At last, by using the LaSalle invariance principle, the convergence theorem is proved.

By means of ω designed in (15) and $v_k(t)$ designed in (16), one can obtain

$$\dot{V} = 0 \Leftrightarrow \Im(\langle \langle \psi | \psi'_{f, \gamma_1, \dots, \gamma_r} \rangle \rangle) = 0, \Im(\langle \langle \psi'_{f, \gamma_1, \dots, \gamma_r} | H_k | \psi \rangle \rangle) = 0. \quad (17)$$

Without loss of generality, assume $\dot{V}(t) = 0, (t \geq t_0)$. After the time t_0 , $\dot{V}(t) = 0$ holds, V is constant, thus $\gamma_k, (k = 1, 2, \dots, r)$ are constants, denoted by $\gamma_k = \bar{\gamma}_k$.

By means of (17) and ignoring higher order terms of dt in the Taylor expansion formula of the state at the time t_0 , $t_1 = t_0 + dt, t_2 = t_1 + dt, \dots$, we can obtain in turn:

$$t_0 : \Im(\langle \langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | \psi(t_0) \rangle \rangle) = 0, \quad (18)$$

$$\Im(\langle \langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | H_k | \psi(t_0) \rangle \rangle) = 0$$

$$t_1 : \Im(\langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | \psi(t_0 + dt) \rangle) = \Im(\langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | \psi(t_0) \rangle) = 0, \quad (19)$$

$$\begin{aligned} \Im(i \langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | [H_{03}, H_k] | \psi(t_0) \rangle) &= 0. \\ &\vdots \\ \Im(\langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | \psi(t_0) \rangle) &= 0, \\ \Im(i^n \langle \psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | [H_{03}^{(n)}, H_k] | \psi(t_0) \rangle) &= 0, (n = 0, 1, \dots), \end{aligned} \quad (20)$$

where $H_{03} = H_0 + \sum_{k=1}^r H_k(\bar{\gamma}_k + \eta_k)$ and

$$[H_{03}^{(n)}, H_k] = \underbrace{[H_{03}, [H_{03}, \dots, [H_{03}, H_k]]]}_{n \text{ times}}. \quad \text{Set}$$

$U = (\phi'_{1, \gamma_1, \dots, \gamma_r}, \dots, \phi'_{N, \gamma_1, \dots, \gamma_r})$, then the system in the eigenbasis of H_{03} is

$$i \dot{\bar{\psi}}(t) = (\bar{H}_0 + \sum_{k=1}^r \bar{H}_k(\gamma_k(t) + v_k(t) + \eta_k) + \omega I) \bar{\psi}(t), \quad (21)$$

where

$$|\psi(t)\rangle = U |\bar{\psi}(t)\rangle, H_0 = U \bar{H}_0 U^\dagger, H_k = U \bar{H}_k U^\dagger. \quad (22)$$

Denote $|\bar{\psi}'_{f, \gamma_1, \dots, \gamma_r}\rangle = U_1^\dagger |\psi'_{f, \gamma_1, \dots, \gamma_r}\rangle$. Substituting (22) into (20) gives

$$\begin{aligned} \Im(\langle \bar{\psi}'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | \bar{\psi}(t_0) \rangle) &= 0, \\ \Im(i^n \langle \bar{\psi}'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | [(\bar{H}_{03})^{(n)}, \bar{H}_k] | \bar{\psi}(t_0) \rangle) &= 0, (n = 0, 1, 2, \dots), \end{aligned} \quad (23)$$

where

$$\bar{H}_{03} = (\bar{H}_0 + \sum_{k=1}^r \bar{H}_k(\bar{\gamma}_k + \eta_k)) = \text{diag}[\lambda'_{1, \bar{\gamma}_1, \dots, \bar{\gamma}_r}, \dots, \lambda'_{N, \bar{\gamma}_1, \dots, \bar{\gamma}_r}].$$

Set $|\bar{\psi}(t_0)\rangle = [\psi_1, \dots, \psi_N]^T$. By condition i), the spectrum of H_{03} is not degenerate, then N eigenstates of \bar{H}_{03} can be written as $[1, 0, \dots, 0]^T, \dots,$ and $[0, 0, \dots, 1]^T$. For convenience, assume $|\bar{\psi}'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r}\rangle = [0, 0, \dots, 1]^T$. Then (23) can be written as

$$\begin{aligned} \Im(\langle \bar{\psi}'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r} | \bar{\psi}(t_0) \rangle) &= 0, \\ \Im(i^n \sum_{j=1}^N (\lambda'_{N, \bar{\gamma}_1, \dots, \bar{\gamma}_r} - \lambda'_{j, \bar{\gamma}_1, \dots, \bar{\gamma}_r})^n (\bar{H}_k)_{Nj} \psi_j) &= 0. \end{aligned} \quad (24)$$

Set

$$\xi = [(\bar{H}_k)_{N1} \psi_1, (\bar{H}_k)_{N2} \psi_2, \dots, (\bar{H}_k)_{NN-1} \psi_{N-1}]^T, \quad (25a)$$

$$\Lambda = \text{diag}[\omega'_{N,1, \bar{\gamma}_1, \dots, \bar{\gamma}_r}, \dots, \omega'_{N,(N-1), \bar{\gamma}_1, \dots, \bar{\gamma}_r}], \quad (25b)$$

$$M = \begin{bmatrix} 1 & \dots & 1 \\ \omega'_{N,1, \bar{\gamma}_1, \dots, \bar{\gamma}_r}{}^2 & \dots & \omega'_{N,(N-1), \bar{\gamma}_1, \dots, \bar{\gamma}_r}{}^2 \\ \vdots & \vdots & \vdots \\ \omega'_{N,1, \bar{\gamma}_1, \dots, \bar{\gamma}_r}{}^{2(N-2)} & \dots & \omega'_{N,(N-1), \bar{\gamma}_1, \dots, \bar{\gamma}_r}{}^{2(N-2)} \end{bmatrix}. \quad (25c)$$

By condition i) and ii), one can obtain

$$\psi_j = 0, (j = 1, \dots, N-1). \quad (26)$$

Therefore (20) is equivalent to

$$|\bar{\psi}(t_0)\rangle = \psi_N |\bar{\psi}'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r}\rangle = e^{i\theta} |\bar{\psi}'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r}\rangle. \quad (27)$$

Thus one can obtain

$$|\psi(t_0)\rangle = e^{i\theta} |\psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r}\rangle. \quad (28)$$

If $\gamma_k(e^{i\theta} |\psi'_{f, \bar{\gamma}_1, \dots, \bar{\gamma}_r}\rangle) = 0$, then

$$|\psi(t_0)\rangle = e^{i\theta} |\psi_f\rangle \quad (29)$$

holds.

According to the LaSalle invariance principle [10], as $t \rightarrow \infty$, any state trajectory of the control system will converge toward $E = \{|\psi\rangle = e^{i\theta} |\psi_f\rangle, \theta \in R\}$. Theorem 1 is proved.

IV. RELATION BETWEEN TWO LYAPUNOV FUNCTIONS

In the Liouville space, the Hilbert-Schmidt distance between two density operators ρ_1 and ρ_2 is

$$d_{HS}(\rho_1, \rho_2) = \sqrt{\text{tr}(\rho_1 - \rho_2)^2}. \quad (30)$$

The inner product of two operators A and B is defined as $\langle\langle A | B \rangle\rangle = \text{tr}(A^\dagger B)$, where the operation A^\dagger refers to the conjugate transpose of A . And by $\rho = |\psi\rangle\langle\psi|$, the square of the Hilbert-Schmidt distance between the density operator ρ and the target density operator $\rho_{f, \gamma_1, \dots, \gamma_r}$ is

$$d_{HS}^2(\rho, \rho_{f, \gamma_1, \dots, \gamma_r}) = 2(1 - |\langle\psi | \psi'_{f, \gamma_1, \dots, \gamma_r}\rangle|^2). \quad (31)$$

By (31) and the implicit Lyapunov functions based on the

state distance $V(\psi) = \frac{1}{2}(1 - \langle \psi | \psi'_{f,\gamma_1,\dots,\gamma_r} \rangle)^2$ [8] and the state

error $V(|\psi\rangle) = \frac{1}{2} \langle \psi - \psi'_{f,\gamma_1,\dots,\gamma_r} | \psi - \psi'_{f,\gamma_1,\dots,\gamma_r} \rangle$ used in this paper, we can conclude that two implicit Lyapunov functions are equivalent in the sense of replacing the pure states with their equivalent density operators.

V. NUMERICAL SIMULATIONS

In this section, a 4-level multi-control Hamiltonians quantum system in a degenerate case is considered. The experiment is done to verify the effectiveness of the implicit Lyapunov control method proposed in this paper, and compare the control effectiveness of implicit Lyapunov control based on the state error with that of the state distance in [8].

In the numerical simulation experiment, the Hamiltonians of the selected 4-level quantum system are

$$H_0 = \text{diag}(1.1, 1.83, 2.56, 3.05),$$

$$H_1 = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, H_2 = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}. \quad (32)$$

Assume the initial state is a superposition state: $|\psi_0\rangle = 0.5(1 \ 1 \ 1 \ 1)^T$, and the target state is an eigenstate: $|\psi_f\rangle = (0 \ 0 \ 0 \ 1)^T$.

According to the design idea proposed in this paper, control laws based on the state error are $u_k(t) = \gamma_k(t) + v_k(t) + \eta_k$, ($k=1,2$) and ω . The implicit functions $\gamma_k(t)$, ($k=1,2$) are designed according to Lemma 1 as $\gamma_k(|\psi\rangle) = \theta_k \left(\frac{1}{2} \langle \psi - \psi'_{f,\gamma_1,\gamma_2} | \psi - \psi'_{f,\gamma_1,\gamma_2} \rangle \right)$, ($k=1,2$), where $\theta_1(s) = C_1 s$, and $\theta_2(s) = C_2 s$. According to (3), η_k are designed as $\eta_1 = \eta_2 = 0$. The control fields $v(t)$ are designed according to (12) as $v_1(t) = K_1 \Im(\langle \psi'_{f,\gamma_1,\gamma_2} | H_1 | \psi \rangle)$, $v_2(t) = K_2 \Im(\langle \psi'_{f,\gamma_1,\gamma_2} | H_2 | \psi \rangle)$. ω is designed according to (11) as: $\omega = -\lambda'_{\gamma_1,\gamma_2} + c \Im(\langle \psi'_{f,\gamma_1,\gamma_2} | \psi \rangle)$. After tuning these control parameters repeatedly and carefully, we choose the control parameters as: $C_1 = 0.04$, $C_2 = 0.02$, $K_1 = 0.3$, $K_2 = 0.7$ and $c = 0.16$.

In the numerical simulation experiment, the sample step is set to be 0.01 a.u., and the control duration is 50 a.u.. Results of the numerical simulation experiment are shown in Figs. 1, 2 and 3. Fig. 1 is the population evolution curves of the control system, $|c_i|^2$, ($i=1,2,3,4$) is the population of level $|i\rangle$ Fig. 2 shows the designed control fields $u_1(t)$ and $u_2(t)$. Fig. 3 shows the designed ω .

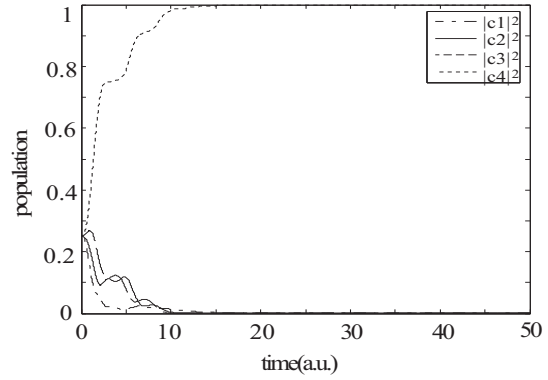


Fig. 1 Populations of four energy levels

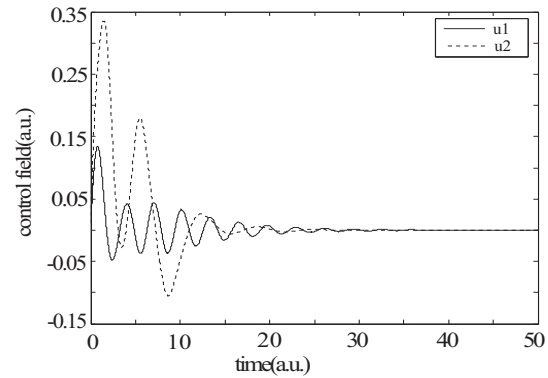


Fig. 2 Control fields $u_1(t)$ and $u_2(t)$

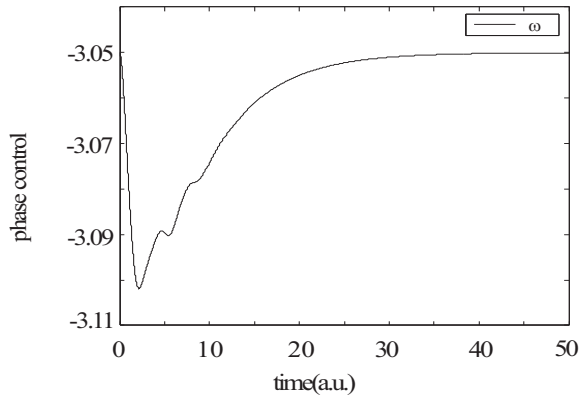


Fig. 3 Imaginary control field ω

One can see from Fig. 1 that at the time 31 a.u., the populations of four energy levels are: $|c_1|^2 = 2.4334 \times 10^{-5}$, $|c_2|^2 = 1.1384 \times 10^{-6}$, $|c_3|^2 = 2.6292 \times 10^{-7}$, and $|c_4|^2 = 0.99997$, respectively. And the transition probability is 99.997%. In the numerical simulation experiment of [8], the same multi-control Hamiltonians quantum system and an implicit Lyapunov control based on the state distance were applied. Results of the numerical simulation experiment in [8]

are: at the time 31 a.u., the populations of four energy levels are: $|c_1|^2 = 2.9111 \times 10^{-7}$, $|c_2|^2 = 8.9707 \times 10^{-6}$, $|c_3|^2 = 8.841 \times 10^{-7}$ and $|c_4|^2 = 0.99999$, respectively. The shortest time that the transition probability is maintained above 99.999% by using the state error method is 35 a.u., and that of the state distance method in [8] is 31 a.u.

From the comparison of numerical simulation experiments, one can see that the proposed implicit Lyapunov control method in this paper is effective. And at a fixed specific time, the transition probability in the case of using the implicit Lyapunov control method based on the state distance is a little better than that in the case of using the implicit Lyapunov control method based on the state error method in the numerical simulation given in this section. As being discussed the relationship, the transition probabilities of these two methods have the same order of magnitude. They have the similar control effect according to the analysis in Section IV.

VI. CONCLUSION

In this paper, according to the basic idea of the implicit Lyapunov control method, a convergent Lyapunov control method based on the state error has been proposed. The proposed method is also suitable for multi-control Hamiltonian systems, the degenerate cases and the case that the target state is a superposition state. In the degenerate cases, the multi-control Hamiltonian system can converge to any pure target state from any pure initial state. The experimental results have indicated that the proposed implicit Lyapunov control method based on the state error is effective, and the control effect of the implicit Lyapunov control methods based on the state distance and that of the state error are basically the same.

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