

Quantum Lyapunov Control Based on the Average Value of an Imaginary Mechanical Quantity

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Abstract: The convergence of closed quantum systems in the degenerate cases to the arbitrary desired target state by using the quantum Lyapunov control based on the average value of an imaginary mechanical quantity is studied in this paper. On the basis of the existing methods which can only ensure the pure states and single-control Hamiltonian systems converge toward a set, we propose a control laws design to make the multi-control Hamiltonian systems, which can also converge from the arbitrary initial state to the arbitrary target state of the quantum systems whose internal Hamiltonian are not strongly regular or/and control Hamiltonians are not full connected. The degenerate cases' problems solved in this paper widely exist in the practical quantum systems, so it has the great significance in quantum systems control. People can make use of those conditions obtained to design a convergent controller for the quantum control system, which can instruct the experimental scientists to obtain high successful probability to the actual quantum systems control. This research work establishes a completed quantum Lyapunov control theory in closed quantum systems. The convergence of the control system is proved. How to make the convergence conditions to be satisfied is proved or analyzed. Finally, numerical simulations for a three level system in the degenerate case transferring from an initial eigenstate to a target superposition state are studied.

Keywords: quantum Lyapunov control method, convergence, degenerate

1. INTRODUCTION

In the last 30 years, the control theory of quantum systems has developed rapidly. Many quantum control methods have been developed such as quantum optimal control (Schmidt, *et al.* 2011), adiabatic control (Boscain, *et al.* 2012), quantum control method based on the Lyapunov stability theorem (Grivopoulos and Bamieh, 2003; Mirrahimi, *et al.* 2005, Kuang, and Cong, 2008), optimal Lyapunov-based quantum control (Hou, *et al.* 2012). Like quantum optimal control theory, the quantum Lyapunov control is also a very powerful control method which uses the Lyapunov indirect stability theorem to design a stable controller. Unlike it used in the macroscopic engineering field, quantum Lyapunov controller should be designed as a convergent one in order to guarantee the control system to achieve the target goal in 100% probability. To do so, the selection of the Lyapunov function is the key point. Up to now, there are mainly three Lyapunov functions to be selected: the Lyapunov function based on the state distance, the state error and the average value of an imaginary mechanical quantity. The former two Lyapunov functions are only suitable for the Schrödinger equation which can only control the pure states, while the Lyapunov function based on the average value of an imaginary mechanical quantity can be used in not only the Schrödinger equation but also quantum Liouville equation which has wider application ranges, and because there is one more tunable coefficient: an imaginary mechanical quantity in the control laws, the control performances become more accuracy or faster convergent rate. The so-called “imaginary

mechanical quantity” means that it is a linear Hermitian operator to be designed and maybe not a physically meaningful observable such as position or energy. In recent years, the research results on the convergence of the control system by using the Lyapunov control method based on the average value of an imaginary mechanical quantity are as follows: The control system is asymptotically stable at the target state, if i) The internal Hamiltonian is strongly regular, i.e., the transition energies between two different levels are clearly identified; ii) The control Hamiltonians are full connected, i.e., any two levels are directly coupled (Wang, and Schirmer, 2010). The systems satisfied above mentioned conditions are called ideal quantum systems or in the non-degenerate cases. However, many practical systems do not satisfy these conditions which are called in the degenerate cases. For these cases, Zhao *et al.* utilized an implicit Lyapunov control to solve the problem of convergence for the single control Hamiltonian systems governed by the Schrödinger equation (Zhao, 2012). However, their proposed methods only proved that the single control Hamiltonian systems will converge toward a set, but can not ensure be asymptotically stable at the desired target state.

The aim of this paper is to make the multi-control Hamiltonian systems in the degenerate cases converge to an arbitrary target state from an arbitrary initial state. The “arbitrary” here means eigenstate, superposition state or mixed state. The main contributions of this paper are as follows: i) The problems of convergence to any target eigenstate for the Schrödinger equation and to any target state which commutes with the internal Hamiltonian for the

quantum Liouville equation are resolved. ii) The problems of convergence to the target superposition state and to the target state which does not commute with the internal Hamiltonian are resolved. iii) How to make the convergence conditions to be satisfied are analyzed or proved. We gave a survey of completed quantum Lyapunov control theory in closed quantum systems in 2010, and 2013, and in this paper we'll give the implicit Lyapunov control convergence conditions proofs in detail, which are suitable for the all kinds of initial and target states in both non-degenerate and degenerate cases.

The paper is arranged as follows: Section 2 is about the convergent control problem solution in the bilinear Schrödinger equation case, in which the existence of the perturbations $\gamma_k(t)$ as a part of control law will be established by Lemma 1. The convergence of the control system is obtained by Theorem 1 based on LaSalle's invariance principle, in detail, the convergence to the eigenstate and superposition state are separately studied. Section 3 is about the quantum Liouville equation case. Section 4 is the numerical simulation of a three-level quantum system in degenerate cases. Section 5 is conclusion.

2. BILINEAR SCHRÖDINGER EQUATION CASE

Consider the N -level closed quantum system governed by the following bilinear Schrödinger equation:

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

where $|\psi(t)\rangle$ is the quantum state vector, H_0 is the internal Hamiltonian, $H_k, (k=1, \dots, r)$ are control Hamiltonians, and $v_k(t), (k=1, \dots, r)$ are control laws.

Two convergence conditions for Hamiltonians have been obtained by Mirrahimi, *et al.* in 2005, Kuang, and Cong in 2008, and Schmidt, *et al.* in 2011 are

i) The internal Hamiltonian is strongly regular, i.e., $\omega_{i'j'} \neq \omega_{lm}, (i', j') \neq (l, m), i', j', l, m \in \{1, 2, \dots, N\}$, where $\omega_{lm} = \lambda_l - \lambda_m$, λ_l is the l -th eigenvalue of H_0 corresponding to the eigenstate $|\phi_l\rangle$;

ii) For any $|\phi_i\rangle \neq |\phi_j\rangle$, there exists at least a k such that $\langle \phi_i | H_k | \phi_j \rangle \neq 0$.

The conditions mentioned above are called ideal quantum systems or in the non-degenerate cases because those conditions basically request in fact the Hamiltonians of system are full-connected which is an ideal situation and seldom appear in the actual quantum system.

In order to solve the convergence problem of the control system in the degenerate cases, a series of (control) perturbations $\gamma_k(t)$, which are implicit functions of state $|\psi(t)\rangle$ and time t , are introduced into the control laws, then the controlled system (1) becomes

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

where $\gamma_k(t) + v_k(t) = u_k(t), (k=1, \dots, r)$ are the total control laws.

Our control task is to make the control system governed by (2) transfer from an arbitrary initial pure state $|\psi_0\rangle$ to an arbitrary target pure state $|\psi_f\rangle$ by designing appropriate combination control laws $u_k(t) = \gamma_k(t) + v_k(t), (k=1, \dots, r)$. In order to so, we need to complete three control tasks: firstly, the control perturbations $\gamma_k(t)$ and control law $v_k(t)$ are designed separately. Secondly, the convergence of the control system is proved. Thirdly, how to make convergence conditions to be satisfied is analyzed.

At first, let us design the control perturbations $\gamma_k(t), (k=1, \dots, r)$. After introducing this control perturbations $\gamma_k(t)$, the combination term

$H_0 + \sum_{k=1}^r H_k \gamma_k(t)$ can be regarded as the new internal Hamiltonian of the control system. In order to facilitate understanding the basic idea of this method, we describe the system in the eigenbasis of $H_0 + \sum_{k=1}^r H_k \gamma_k(t)$ as:

$$i|\dot{\hat{\psi}}(t)\rangle = ((\hat{H}_0 + \sum_{k=1}^r \hat{H}_k \gamma_k(t)) + \sum_{k=1}^r \hat{H}_k v_k(t))|\hat{\psi}(t)\rangle, \quad (3)$$

where $|\hat{\psi}\rangle = U_1^\dagger |\psi\rangle$, $\hat{H}_0 = U_1^\dagger H_0 U_1, \hat{H}_k = U_1^\dagger H_k U_1$, $U_1 = (|\phi_{1,\gamma_1, \dots, \gamma_r}\rangle, \dots, |\phi_{N,\gamma_1, \dots, \gamma_r}\rangle)$, $|\phi_{n,\gamma_1, \dots, \gamma_r}\rangle, 1 \leq n \leq N$ are eigenstates of $H_0 + \sum_{k=1}^r H_k \gamma_k(t)$ corresponding to the eigenvalues $\lambda_{n,\gamma_1, \dots, \gamma_r}$. Accordingly, $|\psi_f\rangle$ will become $|\hat{\psi}_f\rangle = U_1^\dagger |\psi_f\rangle$ which is also a functional of $\gamma_k(t)$.

The aims of designing $\gamma_k(t)$ are two aspects: one to make the control system with $\gamma_k(t)$ become a system in the non-degenerate cases; another is to have the control system with $\gamma_k(t)$ can converge to the arbitrary target state. The first aim requests the $\gamma_k(t)$ must be designed to satisfied the following three conditions: 1) $\gamma_k(t)$ are designed to satisfy i)

$\omega_{l,m,\gamma_1, \dots, \gamma_r} \neq \omega_{i,j,\gamma_1, \dots, \gamma_r}, (l, m) \neq (i, j), i, j, l, m \in \{1, 2, \dots, N\}$ holds, $\omega_{l,m,\gamma_1, \dots, \gamma_r} = \lambda_{l,\gamma_1, \dots, \gamma_r} - \lambda_{m,\gamma_1, \dots, \gamma_r}$; ii) $\forall j \neq l$, for $k=1, \dots, r$, there exists at least a $(\hat{H}_k)_{jl} \neq 0$, where $(\hat{H}_k)_{jl}$

is the (j, l) -th element of \hat{H}_k , thus the control system can converge toward $|\hat{\psi}_f\rangle$ by designing appropriate control laws $u_k(t) = \gamma_k(t) + v_k(t), (k=1, \dots, r)$, thus the control system can converge toward $|\hat{\psi}_f\rangle$ by designing appropriate control laws $u_k(t) = \gamma_k(t) + v_k(t), (k=1, \dots, r)$; 2) at the same time, $\gamma_k(t), (k=1, \dots, r)$ themselves need converge to zero, and their convergent speed must be slower than that of the control system to $|\hat{\psi}_f\rangle$ to make $\gamma_k(t)$ take effect; 3) $\gamma_k(|\psi_f\rangle) = 0$ must hold to make the control system be asymptotically stable at the target state.

For the second design aim, Mirrahimi, *et al.* in 2005, Cong and Meng in 2013 proposed the restriction $V(|\psi_f\rangle) < V(|\psi_0\rangle) < V(|\psi_{other}\rangle)$ to make the system in the non-degenerate cases converge to the target state $|\psi_f\rangle$ from

the initial state $|\psi_0\rangle$, where $|\psi_{other}\rangle$ represents any other state in the invariant set in $E = \{|\psi\rangle | \dot{V}(|\psi\rangle) = 0\}$ except the target state. However, in fact it is difficult to design the imaginary mechanical quantity to make this restriction on the Lyapunov function be satisfied for any initial state and any target state.

For the degenerate cases quantum systems, to make the system converge to the target state, here we choose a simpler restriction: $V(|\psi_f\rangle) < V(|\psi_{other}\rangle)$ which can be satisfied for any initial state and any target state by designing the imaginary mechanical quantity P . In order to ensure the system converge to the target state by adding this restriction, we design all the control perturbations $\gamma_k(t) = 0$ holds for $k = 1, \dots, r$ only at $|\psi_f\rangle$, i.e., 1) $\gamma_k(|\psi_f\rangle) = 0, (k = 1, \dots, r)$, and 2) for $|\psi\rangle \neq |\psi_f\rangle$, there exists at least one k such that $\gamma_k(|\psi\rangle) \neq 0$.

According to the idea analysis mentioned above, let us design the specific $\gamma_k(t), (k = 1, \dots, r)$ in detail. Since the evolution of the system's state relies on the continuous decrease of the Lyapunov function $V(t)$ in the Lyapunov control, we design $\gamma_k(t)$ be a monotonically increasing functional of $V(t)$ as:

$$\gamma_k(|\psi\rangle) = C_k \cdot \theta_k(V(|\psi\rangle) - V(|\psi_f\rangle)), \quad (4)$$

where $C_k \geq 0$, and for $k = 1, \dots, r$, there exists at least a $C_k > 0$. And $\theta_k(\cdot)$ satisfies $\theta_k(0) = 0$, $\theta_k(s) > 0$ and $\theta'_k(s) > 0$ for every $s > 0$.

In this paper the specific Lyapunov function based on the average value of an imaginary mechanical quantity P is selected as:

$$V(|\psi\rangle) = \langle \psi | P_{\gamma_1, \dots, \gamma_r} | \psi \rangle, \quad (5)$$

where $P_{\gamma_1, \dots, \gamma_r} = f(\gamma_1(t), \dots, \gamma_r(t))$ is a functional of $\gamma_k(t)$ and positive definite.

The existence of $\gamma_k(t)$ can be established by Lemma 1.

Lemma 1: If $C_k = 0$, $\gamma_k(|\psi\rangle) = 0$. Else if $C_k > 0$, $\theta_k \in C^\infty(R^+; [0, \gamma_k^*]), k = 1, \dots, r$ (γ_k^* is a positive constant) satisfy $\theta_k(0) = 0$, $\theta_k(s) > 0$ and $\theta'_k(s) > 0$ for every $s > 0$,

$$\text{and } \left| \theta'_k \right| < 1 / (2C_k C^*), \quad C^* = 1 + C,$$

$C = \max \left\{ \left\| \frac{\partial P_{\gamma_1, \dots, \gamma_r}}{\partial \gamma_k} \right\|_\infty, \gamma_k \in [0, \gamma_k^*] \right\}$, then for every $|\psi\rangle \in S^{2N-1}$, there is a unique $\gamma_k \in C^\infty(\gamma_k \in [0, \gamma_k^*])$ satisfying

$$\gamma_k(|\psi\rangle) = C_k \cdot \theta_k(\langle \psi | P_{\gamma_1, \dots, \gamma_r} | \psi \rangle - \langle \psi_f | P_{\gamma_1, \dots, \gamma_r} | \psi_f \rangle) \quad (6)$$

Proof:

Assume $P_{\gamma_1, \dots, \gamma_r}$ are analytic functions of the parameters $\gamma_k(\psi) \in [0, \gamma_k^*], (k = 1, \dots, r)$. $\frac{\partial P_{\gamma_1, \dots, \gamma_r}}{\partial \gamma_k}$ are bounded on $[0, \gamma_k^*]$, thus $C < \infty$. Define

$$F_k(\gamma_1, \dots, \gamma_r, |\psi\rangle) = \gamma_k - C_k \cdot \theta_k(\langle \psi | P_{\gamma_1, \dots, \gamma_r} | \psi \rangle - \langle \psi_f | P_{\gamma_1, \dots, \gamma_r} | \psi_f \rangle)$$

where $F_k(\gamma_1, \dots, \gamma_r, |\psi\rangle)$ are regular. For a fixed $|\psi\rangle$, $F_k(\gamma_1(|\psi\rangle), \dots, \gamma_r(|\psi\rangle), |\psi\rangle) = 0$ holds. Some deductions show that $\frac{\partial F_k(\gamma_1, \dots, \gamma_r, |\psi\rangle)}{\partial \gamma_k} \neq 0$ holds. Thus according to the implicit function Theorem [11], Lemma 1 is proved. \square

Remark 1: For the sake of simplicity, set $\gamma_k(t) = 0$ for some k , and other $\gamma_k(t)$ are equal, denoted by $\gamma(t)$, i.e., set

$$\gamma_k(t) = \gamma(t) = \theta(\langle \psi | P_\gamma | \psi \rangle - \langle \psi_f | P_\gamma | \psi_f \rangle), k = k_1, \dots, k_m; \quad (7)$$

$$\gamma_k(t) = 0, k \neq k_1, \dots, k_m (1 \leq k_1, \dots, k_m \leq r),$$

where $\theta(\cdot) = \theta_{k_1}(\cdot) = \dots = \theta_{k_m}(\cdot)$ and P_γ are functions of $\gamma(t)$.

Then let us design another control law $v_k(t)$ to make $\dot{V}(t) \leq 0$ holds. Setting $[P_\gamma, H_0 + \sum_{n=k_1}^{k_m} H_n \gamma(t)] = 0$, one can obtain the time derivative of the selected Lyapunov function as:

$$\begin{aligned} \dot{V} = & \sum_{k=1}^r i v_k(t) \langle \psi | [H_k, P_\gamma] | \psi \rangle \cdot (1 + \theta'(\langle \psi_f | (\frac{\partial P_\gamma}{\partial \gamma}) | \psi_f \rangle)) \\ & / (1 - \theta'(\langle \psi | (\frac{\partial P_\gamma}{\partial \gamma}) | \psi \rangle - \langle \psi_f | (\frac{\partial P_\gamma}{\partial \gamma}) | \psi_f \rangle)). \end{aligned} \quad (8)$$

According to Lemma 1, one can obtain $(1 + \theta'(\langle \psi_f | (\frac{\partial P_\gamma}{\partial \gamma}) | \psi_f \rangle)) / (1 - \theta'(\langle \psi | (\frac{\partial P_\gamma}{\partial \gamma}) | \psi \rangle - \langle \psi_f | (\frac{\partial P_\gamma}{\partial \gamma}) | \psi_f \rangle)) > 0$ holds. In order to ensure $\dot{V}(t) \leq 0$, $v_k(t), (k = 1, \dots, r)$ are designed as:

$$v_k(t) = -K_k f_k(i \langle \psi | [H_k, P_\gamma] | \psi \rangle), (k = 1, \dots, r) \quad (9)$$

where K_k is a constant and $K_k > 0$, and $y_k = f_k(x_k), (k = 1, 2, \dots, r)$ are monotonic increasing functions through the coordinate origin of the plane $x_k - y_k$.

Based on LaSalle's invariance principle (LaSalle and Lefschetz, 1961), the convergence of the control system governed by (2) can be obtained as follows:

Theorem 1: Consider the control system governed by (2) with the combination control fields $u_k(t) = \gamma_k(t) + v_k(t), (k = 1, \dots, r)$, where $\gamma_k(t)$ defined by Lemma 1 and (7), and $v_k(t)$ defined by (9). If the control system satisfies:

$$i) \quad \omega_{l,m,\gamma} \neq \omega_{i,j,\gamma}, (l,m) \neq (i,j), \quad i, j, l, m \in \{1, 2, \dots, N\},$$

$$\omega_{l,m,\gamma} = \lambda_{l,\gamma} - \lambda_{m,\gamma}, \text{ where } \lambda_{l,\gamma} \text{ is the } l\text{-th eigenvalue of } H_0 + \sum_{n=k_1}^{k_m} H_n \gamma(t) \text{ corresponding to the eigenstate } |\phi_{l,\gamma}\rangle;$$

$$ii) \text{ For any } i \neq j, i, j \in \{1, 2, \dots, N\}, \text{ there exists at least one } k \text{ such that } (\hat{H}_k)_{lm} \neq 0, \text{ where } (\hat{H}_k)_{lm} \text{ is the } (l,m)\text{-th element of } \hat{H}_k = U_1^\dagger H_k U_1, U_1 = (|\phi_{1,\gamma}\rangle, \dots, |\phi_{N,\gamma}\rangle);$$

$$iii) [P_\gamma, H_0 + \sum_{n=k_1}^{k_m} H_n \gamma(t)] = 0;$$

iv) $(\hat{P}_\gamma)_{ll} \neq (\hat{P}_\gamma)_{mm}, l \neq m$, where $(\hat{P}_\gamma)_{ll}$ is the (l,l) -th element of $U_1^\dagger P_\gamma U_1$.

then any trajectory will converge toward $E_1 = \left\{ |\psi_{t_0}\rangle \left| e^{i\theta_l} \left| \phi_{l,\gamma}(|\psi_{t_0}\rangle) \right. \right. \right\}; \theta_l \in R, l \in \{1, \dots, N\}$.

Proof:

Without loss of generality, assume that for $t \geq t_0, (t_0 \in R)$, $\dot{V} = 0$ is satisfied. By (8) and (9), one obtains

$$\dot{V} = 0 \Leftrightarrow \langle \psi | [H_k, P_\gamma] | \psi \rangle = 0 \Leftrightarrow v_k(t) = 0 \quad (10)$$

As $\dot{V} = 0$, γ is a constant, denoted by $\bar{\gamma}$. The state $|\psi(t_0)\rangle$ can be written as $|\psi(t_0)\rangle = \sum_{l=1}^N c_l(t_0) |\phi_{l,\bar{\gamma}}\rangle$. Then $|\hat{\psi}(t_0)\rangle$ can be written as $|\hat{\psi}(t_0)\rangle = \sum_{l=1}^N c_l(t_0) U_1^H |\phi_{l,\bar{\gamma}}\rangle$. Substituting the solution of (3) with $\gamma = \bar{\gamma}$ and $v_k(t) = 0$ into $\langle \hat{\psi} | [\hat{H}_k, \hat{P}_\gamma] | \hat{\psi} \rangle = \langle \psi | [H_k, P_\gamma] | \psi \rangle = 0$, gives

$$\sum_{l,m=1}^N e^{i\omega_{l,m,\bar{\gamma}}(t-t_0)} \left((\hat{P}_{\bar{\gamma}})_{mm} - (\hat{P}_{\bar{\gamma}})_{ll} \right) c_l^*(t_0) c_m(t_0) (\hat{H}_k)_{lm} = 0 \quad (11)$$

By conditions i)-ii) and iv), one can have

$$c_l^*(t_0) c_m(t_0) = 0, (l, m \in \{1, \dots, N\}) \quad (12)$$

which implies that there is at most one $c_l(t_0) (l \in \{1, \dots, N\})$ which is nonzero. Theorem 1 is proved. □

Remark 2: Theorem 1 guarantees the control system to converge to the set E_1 , however, it can not guarantee the control system converges to the target state. So the following we'll study how to make the control system convergen to the target state contained in E_1 , which needs to be discussed in the cases of target state being an eigenstate or a superposition state separately.

2.1 In the case of target state being an eigenstate

From Theorem 1, one can see that if the target state $|\psi_f\rangle$ is an eigenstate, $|\psi_f\rangle$ is contained in E_1 because of $\gamma(|\psi_f\rangle) = 0$. In order to make the system converge to the target state, on the one hand, as $\dot{V} \leq 0$, we design P_γ to make

$$V(|\psi_f\rangle) < V(|\psi_{other}\rangle) \quad (13)$$

hold, where $|\psi_{other}\rangle$ represents any other state in the set E_1 except the target state. On the other hand, because $\partial\gamma / \partial V > 0, \dot{V} \leq 0, \gamma \geq 0$ holds, we set $\gamma = \bar{\gamma} - \alpha, (0 < \alpha \ll \bar{\gamma})$ when $v_k(t) = 0, \gamma(t) = \bar{\gamma} \neq 0$ holds for some time to make the state trajectory evolve but not stay in E_1 until $|\psi_f\rangle e^{i\theta_l}$, which is the equivalent state of target state $|\psi_f\rangle$, is reached.

From the above analysis, we can see that if the control system satisfies the conditions i)-iv) in Theorem 1 and Eq.(13), and at the same time set $\gamma = \bar{\gamma} - \alpha, (0 < \alpha \ll \bar{\gamma})$ when $v_k(t) = 0, \gamma(t) = \bar{\gamma} \neq 0$ holds for some time, the control system (2) can converge to the target eigenstate from an arbitrary initial pure state.

Next we'll analyze how to make these conditions be satisfied in detail. Conditions i) and ii) in Theorem 1 are associated with $H_0, H_k, (k=1, \dots, r)$ and $\gamma_k(t)$. By designing appropriate $\gamma_k(t)$, these two conditions can be satisfied in most cases. Condition iii) means that P_γ and $H_0 + \sum_{n=k_1}^{k_m} H_n \gamma(t)$ have the same eigenstates. We design the eigenvalues of P_γ be constant, denoted by P_1, P_2, \dots, P_N , and design P_γ as

$$P_\gamma = \sum_{j=1}^N P_j |\phi_{j,\gamma}\rangle \langle \phi_{j,\gamma}| \quad (14)$$

then condition iii) can be satisfied. If design $P_l \neq P_j (\forall l \neq j; 1 \leq l, j \leq N)$ to make condition iv) hold. Then let us analyze how to make (13) hold. The research result is given by the following Theorem 2.

Theorem 2: If one designs $P_i > P_f, (i=1, \dots, N, P_i \neq P_f)$, then $V(|\psi_f\rangle) < V(|\psi_{other}\rangle)$ holds, where P_f is the eigenvalue of $P_\gamma(|\psi_f\rangle)$ corresponding to $|\psi_f\rangle$.

Proof: Set $|\psi_s\rangle = (e^{i\theta_l} |\phi_{l,\bar{\gamma}}\rangle)_{\gamma=0}$. According to Proposition 1 in Zhao in 2012, if one designs $P_i > P_f, (i=1, \dots, N, P_i \neq P_f)$, then $V(|\psi_f\rangle) < V(|\psi_s\rangle)$ holds. Because of $\partial\gamma / \partial V > 0, \dot{V} \leq 0, \gamma > 0$, $V(|\psi_s\rangle) < V(|\psi_{other}\rangle)$ holds. Thus $V(|\psi_f\rangle) < V(|\psi_{other}\rangle)$ holds. Theorem 2 is proved. □

Remark 3: According to the above analysis and Theorem 2, the design principle of the imaginary mechanical quantity is $P_i > P_f, (i=1, \dots, N, P_i \neq P_f)$ and $P_l \neq P_j (\forall l \neq j)$.

2.2 In the case of target state being a superposition state

In order to solve the problem of convergence to the target state being a superposition state, a series of another control disturbances η_k whose values are constant are introduced into the control laws. Thus the equation (2) will become

$$i|\dot{\psi}(t)\rangle = (H_0 + \sum_{k=1}^r H_k(\eta_k + \gamma_k(t) + v_k(t)))|\psi(t)\rangle. \quad (15)$$

Our basic idea is to design η_k to make the target state $|\psi_f\rangle$ be an eigenstate of $H'_0 = H_0 + \sum_{k=1}^r H_k \eta_k$. H'_0 can be viewed as the new internal Hamiltonian of the control system. If the number of the control Haimltonians r is large enough, by designing appropriate η_k , $(H_0 + \sum_{k=1}^r H_k \eta_k) |\psi_f\rangle = \lambda'_f |\psi_f\rangle$ can be satisfied in most cases, where λ'_f is the eigenvalue of H'_0 corresponding to $|\psi_f\rangle$. Then the design of control laws and the convergence proof can follow the target eigenstate cases. One can prove that the designed control laws are also valid and Theorem 1 and Theorem 2 also holds with changing H_0 into H'_0 .

3. QUANTUM LIOUVILLE EQUATION CASE

Consider the N -level closed quantum system governed by the following quantum Liouville equation:

$$i\dot{\rho}(t) = [H_0 + \sum_{k=1}^r H_k(\gamma_k(t) + v_k(t) + \eta_k), \rho(t)], \quad (16)$$

where $\gamma_k(t) + v_k(t) + \eta_k = u_k(t), (k=1, \dots, r)$ are the total control laws.

The design ideas are similar to that of Section 2. The specific Lyapunov function is selected as:

$$V(\rho) = \text{tr}(P_{\gamma_1, \dots, \gamma_r} \rho), \quad (17)$$

where $P_{\gamma_1, \dots, \gamma_r} = f(\gamma_1(t), \dots, \gamma_r(t))$ is a functional of $\gamma_k(t)$ and positive definite.

For the sake of simplicity, design $\gamma_k(t)$ as

$$\gamma_k(t) = \gamma(t) = \theta(V(\rho) - V(\rho_f)), k = k_1, \dots, k_m; \quad (18)$$

$$\gamma_k(t) = 0, k \neq k_1, \dots, k_m (1 \leq k_1, \dots, k_m \leq r),$$

where $\theta(\cdot)$ satisfies $\theta(0) = 0$, $\theta(s) > 0$ and $\theta'(s) > 0$ for every $s > 0$. Accordingly, $P_{\gamma_1, \dots, \gamma_r}$ becomes P_γ . The existence of $\gamma(t)$ can be depicted by Lemma 2.

Lemma 2: If $\theta \in C^\infty(R^+; [0, \gamma^*]), k=1, \dots, r$ (γ^* is a positive constant) satisfy $\theta(0) = 0$, $\theta(s) > 0$ and $\theta'(s) > 0$ for every $s > 0$, and $|\theta'| < 1/(2C^*)$, $C^* = 1 + C$,

$$C = \max \left\{ \left\| \frac{\partial P_\gamma}{\partial \gamma} \right\|_{m_1}, \gamma \in [0, \gamma^*] \right\},$$

then for every ρ , there is a unique $\gamma \in C^\infty(\gamma \in [0, \gamma^*])$ satisfying $\gamma(\rho) = \theta(\text{tr}(P_\gamma \rho) - \text{tr}(P_\gamma \rho_f))$.

The idea of proof is similar to that of Lemma 1 in Section 2.

Then let us design $v_k(t)$ such that $\dot{V}(t) \leq 0$ holds. Setting

$$[P_\gamma, H_0 + \sum_{k=1}^r H_k \eta_k + \sum_{n=k_1}^{k_m} H_n \gamma(t)] = 0, \text{ one can obtain}$$

$$\dot{V} = -(1 + \theta' \text{tr}((\partial P_\gamma / \partial \gamma) \rho_f)) / (1 - \theta' \text{tr}((\partial P_\gamma / \partial \gamma)(\rho - \rho_f))) \cdot \sum_{k=1}^r \text{itr}(P_\gamma, H_k \rho) v_k(t) \quad (19)$$

By $|\theta'| < 1/(2C^*)$ in Lemma 2,

$$(1 + \theta' \text{tr}((\partial P_\gamma / \partial \gamma) \rho_f)) / (1 - \theta' \text{tr}((\partial P_\gamma / \partial \gamma)(\rho - \rho_f))) > 0$$

holds. In order to ensure $\dot{V}(t) \leq 0$, $v_k(t), (k=1, \dots, r)$ are designed as:

$$v_k(t) = K_k f_k(\text{itr}(P_\gamma, H_k \rho)), (k=1, \dots, r), \quad (20)$$

where K_k is a constant and $K_k > 0$, and $y_k = f_k(x_k), (k=1, 2, \dots, r)$ are monotonic increasing functions which are through the coordinate origin of the plane $x_k - y_k$.

Based on LaSalle's invariance principle, the convergence of the control system can be obtained as follows.

Theorem 3: Consider the control system depicted by (16) with control laws $\gamma_k(t)$ defined by Lemma 2 and Eq. (18), and $v_k(t)$ defined by (20). If the control system satisfies:

- i) $\omega_{l,m,\gamma} \neq \omega_{i,j,\gamma}, (l,m) \neq (i,j), i,j,l,m \in \{1, 2, \dots, N\}$,
 $\omega_{l,m,\gamma} = \lambda_{l,\gamma} - \lambda_{m,\gamma}$, where $\lambda_{l,\gamma}$ is the l -th eigenvalue of

$H_0 + \sum_{k=1}^r H_k \eta_k + \sum_{n=k_1}^{k_m} H_n \gamma(t)$ corresponding to the eigenstate $|\phi_{l,\gamma}\rangle$;

- ii) $\forall j \neq l$, for $k=1, \dots, r$, there exists at least a $(\hat{H}_k)_{jl} \neq 0$,

where $(\hat{H}_k)_{jl}$ is the (j,l) -th element of $\hat{H}_k = U_2^\dagger H_k U_2$

with $U_2 = (|\phi_{1,\gamma}\rangle, \dots, |\phi_{N,\gamma}\rangle)$;

- iii) $[P_\gamma, H_0 + \sum_{k=1}^r H_k \eta_k + \sum_{n=k_1}^{k_m} H_n \gamma(t)] = 0, 1 \leq k_1, \dots, k_m \leq r$;

- iii) For any $l \neq j, (1 \leq l, j \leq N)$, $(\hat{P}_\gamma)_{ll} \neq (\hat{P}_\gamma)_{jj}$ holds,

where $(\hat{P}_\gamma)_{ll}$ is the (l,l) -th element of $\hat{P}_\gamma = U_2^\dagger P_\gamma U_2$.

then the control system will converge toward

$$E_2 = \left\{ \rho_{t_0} \mid (U_2^\dagger \rho_{t_0} U_2)_{ij} = 0, \gamma = \gamma(\rho_{t_0}), t_0 \in R \right\}.$$

Proof:

Without loss of generality, assume that for $t \geq t_0, (t_0 \in R)$, $\dot{V} = 0$ is satisfied. By (19) and (20), one can get

$$\dot{V} = 0 \Leftrightarrow \text{tr}([P_\gamma, H_k] \rho) = 0 \Leftrightarrow v_k(t) = 0 \quad (21)$$

As $\dot{V} = 0$, γ are constants, denoted by $\bar{\gamma}$. The control system in the eigenbasis of

$H_0 + \sum_{k=1}^r H_k \eta_k + \sum_{n=k_1}^{k_m} H_n \gamma(t)$ is

$$i\dot{\hat{\rho}}(t) = [(\hat{H}_0 + \sum_{k=1}^r \hat{H}_k(\gamma_k(t) + \eta_k)) + \sum_{k=1}^r \hat{H}_k v_k(t), \hat{\rho}(t)] \quad (22)$$

where $\hat{\rho} = U_2^\dagger \rho U_2, \hat{H}_0 = U_2^\dagger H_0 U_2, \hat{H}_k = U_2^\dagger H_k U_2$. Set $\hat{\rho}_{t_0} = \hat{\rho}(t_0)$. Substituting the solution of Eq. (22) with $\gamma_k(t)$ defined by Eq. (18), $\gamma = \bar{\gamma}$, and $v_k(t) = 0$ into

$\text{tr}([\hat{P}_{\bar{\gamma}}, \hat{H}_k] \hat{\rho}) = \text{tr}([P_\gamma, H_k] \rho) = 0$, gives

$$\text{tr}(e^{-i(\hat{H}_0 + \sum_{k=1}^r \hat{H}_k \eta_k + \sum_{n=k_1}^{k_m} \hat{H}_n \bar{\gamma})(t-t_0)} \hat{\rho}_{t_0} e^{i(\hat{H}_0 + \sum_{k=1}^r \hat{H}_k \eta_k + \sum_{n=k_1}^{k_m} \hat{H}_n \bar{\gamma})(t-t_0)} [\hat{P}_{\bar{\gamma}}, \hat{H}_k]) = 0 \quad (23)$$

where $\hat{P}_{\bar{\gamma}} = U_2^\dagger P_{\bar{\gamma}} U_2$. By condition iii), one can obtain

$$\sum_{j,l=1}^N \omega_{j,l,\bar{\gamma}}^n (\hat{H}_k)_{jl} ((\hat{P}_{\bar{\gamma}})_{ll} - (\hat{P}_{\bar{\gamma}})_{jj}) (\hat{\rho}_{t_0})_{lj} = 0. \quad (24)$$

Set

$$\xi_k = \begin{bmatrix} (\hat{H}_k)_{12} ((\hat{P}_{\bar{\gamma}})_{22} - (\hat{P}_{\bar{\gamma}})_{11}) (\hat{\rho}_{t_0})_{21} \\ \vdots \\ (\hat{H}_k)_{(N-1)N} ((\hat{P}_{\bar{\gamma}})_{NN} - (\hat{P}_{\bar{\gamma}})_{(N-1)(N-1)}) (\hat{\rho}_{t_0})_{N(N-1)} \end{bmatrix}, \quad (25a)$$

$$\Lambda = \text{diag}(\omega_{1,2,\bar{\gamma}}, \dots, \omega_{N-1,N,\bar{\gamma}}), \quad (25b)$$

$$M = \begin{bmatrix} 1 & 1 & \dots & 1 \\ \omega_{1,2,\bar{\gamma}}^2 & \omega_{1,3,\bar{\gamma}}^2 & \dots & \omega_{N,N-1,\bar{\gamma}}^2 \\ \vdots & \vdots & \vdots & \vdots \\ \omega_{1,2,\bar{\gamma}}^{N(N-1)-2} & \omega_{1,3,\bar{\gamma}}^{N(N-1)-2} & \dots & \omega_{N,N-1,\bar{\gamma}}^{N(N-1)-2} \end{bmatrix}. \quad (25c)$$

For $n=0, 2, 4, \dots$, (24) reads $M \Im(\xi_k) = 0$. For $n=1, 3, 5, \dots$,

(24) reads $M\Lambda\Re(\xi_k) = 0$. By condition i), and M and Λ are nonsingular real matrices, one can obtain $\xi_k = 0$. By condition ii) and iv), one have $(\hat{\rho}_{t_0})_{ij} = 0$ holds. Theorem 3 is proved. \square

If r is large enough, by designing appropriate η_k , $[H_0 + \sum_{k=1}^r H_k \eta_k, \rho_f] = 0$ can be satisfied in most cases. Then the target state ρ_f is contained in E_2 . For the special case that the target state commutes with the internal Hamiltonian, i.e., $[\rho_f, H_0] = 0$, set $\eta_k = 0$. Some analyses show that E_2 has at most $N!$ elements. In order to make the system converge to the target state ρ_f , on the one hand, we design P_γ to make

$$V(\rho_f) < V(\rho_{other}) \quad (26)$$

hold, where ρ_{other} represents any other state in the set E_2 except the target state. On the other hand, we design $\gamma = \bar{\gamma} - \alpha$, ($0 < \alpha \ll \bar{\gamma}$) when $v_k(t) = 0, \gamma(t) = \bar{\gamma} \neq 0$ holds for some time to make the state trajectory evolve but not stay in E_2 until ρ_f is reached.

Next we'll analyze how to make these conditions be satisfied. For satisfaction of conditions i) - iv), one can follow that of Section 2. Then let us analyze how to make (26) hold. Denoting the eigenstates of $H_0 + \sum_{k=1}^r H_k \eta_k$ as $|\phi_{i,\eta}\rangle, (i \in \{1, \dots, N\})$, $\tilde{\rho}_f = U_3^\dagger \rho_f U_3$ can be expressed by a diagonal matrix, where $U_3 = (|\phi_{1,\eta}\rangle, \dots, |\phi_{N,\eta}\rangle)$. The research result is as follows:

Theorem 4: If $(\tilde{\rho}_f)_{ii} < (\tilde{\rho}_f)_{jj}, 1 \leq i, j \leq N$, design $P_i > P_j$; if $(\tilde{\rho}_f)_{ii} = (\tilde{\rho}_f)_{jj}, 1 \leq i, j \leq N$, design $P_i \neq P_j$; else if $(\tilde{\rho}_f)_{ii} > (\tilde{\rho}_f)_{jj}, 1 \leq i, j \leq N$, design $P_i < P_j$, then $V(\rho_f) < V(\rho_{other})$ holds, where $(\tilde{\rho}_f)_{ii}$ is the (i,i) -th element of $\tilde{\rho}_f$.

Proof:

At first, propositions 1 and 2 are proposed, then Theorem 4 are proved according to these two propositions.

Proposition 1: If $\{(\tilde{\rho}_f)_{11}, (\tilde{\rho}_f)_{22}, \dots, (\tilde{\rho}_f)_{NN}\}$ arranged in a decreasing order, design $\{P_1, P_2, \dots, P_N\}$ arranged in an increasing order, then $V(\rho_f) < V(\rho_{other})$ holds.

Proof:

Denote $\tilde{\rho}_s = U_3^\dagger \rho_s U_3 = \text{diag}((\tilde{\rho}_f)_{11(\tau)}, (\tilde{\rho}_f)_{22(\tau)}, \dots, (\tilde{\rho}_f)_{NN(\tau)})$, where $\{11(\tau), 22(\tau), \dots, NN(\tau)\}$ is a permutation of $\{11, 22, \dots, NN\}$. At first, we prove $V(\rho_f) < V(\rho_s)$. The Lyapunov function $V(\rho) = \text{tr}(P_\gamma \rho)$ for $\gamma = 0$ can be written as

$$V(\rho)|_{\gamma=0} = \sum_{j=1}^N P_j \tilde{\rho}_{jj}, \quad (27)$$

where $\tilde{\rho}_{jj}$ is the (j,j) -th element of $\tilde{\rho} = U_3^\dagger \rho U_3$. Assume $(\tilde{\rho}_f)_{11} \dots > (\tilde{\rho}_f)_{NN} \geq 0$, and $0 < P_1 < \dots < P_N$. For $N = 2$, $V(\rho_f)_2 - V(\rho_s)_2 = (P_1 - P_2)((\tilde{\rho}_f)_{11} - (\tilde{\rho}_f)_{22}) < 0$, (28) where the subscript "2" in $V(\rho_f)_2$ and $V(\rho_s)_2$ means $N = 2$. Proposition 1 is true.

Assume Proposition 1 is true for $N-1$. Then $V(\rho_f)_{N-1} - V(\rho_s)_{N-1} = \sum_{j=1}^{N-1} P_j ((\tilde{\rho}_f)_{jj} - (\tilde{\rho}_s)_{jj(\tau)}) = \sum_{j=1}^{N-1} (P_{j(\tau)} - P_j) (\tilde{\rho}_f)_{jj(\tau)} < 0$ (29)

where $P_{j(\tau)} = (P_\gamma|_{\gamma=0})_{jj(\tau)}$. For N , $V(\rho_f)_N - V(\rho_s)_N = \sum_{j=1}^{N-1} (P_{j(\tau)} - P_j) (\tilde{\rho}_f)_{jj(\tau)} + (P_{N(\tau)} - P_N) (\tilde{\rho}_f)_{NN(\tau)}$ (30)

By (29) and $0 < P_1 < P_2 < \dots < P_N$, one can get $V(\rho_f)_N - V(\rho_s)_N < 0$ (31)

Because of $\partial\gamma / \partial V > 0, \dot{V} \leq 0, \gamma > 0$, $V(\rho_s) < V(\rho_{other})$ holds. Thus Proposition 1 is proved. \square

Proposition 2: If the diagonal elements of the diagonal target state $\{(\rho_f)_{11}, (\rho_f)_{22}, \dots, (\rho_f)_{NN}\}$ are arranged in a non-decreasing order with $(\rho_f)_{k_{11}k_{11}} = \dots = (\rho_f)_{k_{1L_1}k_{1L_1}} < (\rho_f)_{k_{21}k_{21}} = \dots = (\rho_f)_{k_{2L_2}k_{2L_2}} < \dots < (\rho_f)_{k_{QL}k_{QL}} = \dots = (\rho_f)_{k_{QLQ}k_{QLQ}}$, $1 \leq k_{ij} \leq N, k_{11} = 1, k_{QLQ} = N$

where $i = 1, 2, \dots, Q$, and $j = 1, 2, \dots, L_1$ for $i = 1$; $j = 1, 2, \dots, L_2$ for $i = 2$; \dots ; $j = 1, 2, \dots, L_Q$ for $i = Q$. Design $\{P_1, P_2, \dots, P_N\}$ as follows: $P_{k_{11}}, \dots, P_{k_{1L_1}} > \dots > P_{k_{Q1}}, \dots, P_{k_{QLQ}} > 0$, then $V(\rho_f) < V(\rho_{other})$ holds.

Proof:

Obviously, $V(\rho_f) < V(\rho_s)$ holds for $N=2$. Assume that for $N-1$, $V(\rho_f) < V(\rho_s)$ is true. Then Eq. (29) holds. For N , if $(\tilde{\rho}_f)_{(N-1)(N-1)} < (\tilde{\rho}_f)_{NN}$, design $P_{k_{11}}, \dots, P_{k_{1L_1}} > \dots > P_N$, then (31) holds. If $(\tilde{\rho}_f)_{k_{Q1}k_{Q1}} = (\tilde{\rho}_f)_{k_{Q2}k_{Q2}} = \dots = (\tilde{\rho}_f)_{NN}$, then $NN(\tau) \neq k_{Q1}k_{Q1} \neq \dots \neq k_{Q(L_Q-1)}k_{Q(L_Q-1)}$ in (30). Design $P_{k_{11}}, \dots, P_{k_{1L_1}} > \dots > P_{k_{Q1}}, \dots, P_{k_{QLQ}}$, then (31) holds. Proposition 2 is proved. \square

Obviously, according to Proposition 1 and Proposition 2, we can obtain Theorem 4. \square

4. NUMERICAL SIMULATION

In order to verify the effectiveness of the proposed method, consider a three-level system with H_0 and H_I as:

$$H_0 = \begin{bmatrix} 0.3 & 0 & 0 \\ 0 & 0.5 & 0 \\ 0 & 0 & 0.9 \end{bmatrix}, H_1 = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, H_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix}. \quad (32)$$

According to H_0 and H_1 , the system is in the degenerate case. Assume that the initial state is an eigenstate as

$|\psi_0\rangle = (0 \ 0 \ 1)^T$, and the target state is a superposition state as $|\psi_f\rangle = (\sqrt{2/3} \ -\sqrt{1/3} \ 0)^T$.

According to the design ideas in Section 2, the control law is designed as $u_k(t) = \gamma_k(t) + v_k(t) + \eta_k, (k=1,2)$. Design $\eta_1 = -0.3771, \eta_2 = 0$ to make the target state $|\psi_f\rangle$ be an eigenstate of $H'_0 = H_0 + \sum_{k=1}^2 H_k \eta_k$. H'_0 And design

$$\begin{aligned} \gamma_1 = \gamma_2 = \gamma &= 0.01 \cdot (\langle \psi | P_\gamma | \psi \rangle - \langle \psi_f | P_\gamma | \psi_f \rangle), \\ v_1(t) &= -0.2 \cdot (i \langle \psi | [H_1, P_\gamma] | \psi \rangle), \\ v_2(t) &= -0.2 \cdot (i \langle \psi | [H_2, P_\gamma] | \psi \rangle), \end{aligned}$$

where $P_\gamma = \sum_{j=1}^3 P_j |\phi_{j,\gamma}\rangle$.

According to Theorem 2 in Section 2, set $P_f = 0.1$ and other two eigenvalues of P_γ are 0.4 and 0.6.

In the simulations, the time step size is set as 0.01 a.u., and the control duration is 300 a.u.. The results of numerical simulations are shown in Fig.1 and Fig.2. Fig.1 is the population evolution curves of the control system, $|c_i|^2, (i=1,2,3)$ is the population of level $|i\rangle$. Fig.2 shows the designed control fields. According to numerical results, we can see that the proposed method is effective.

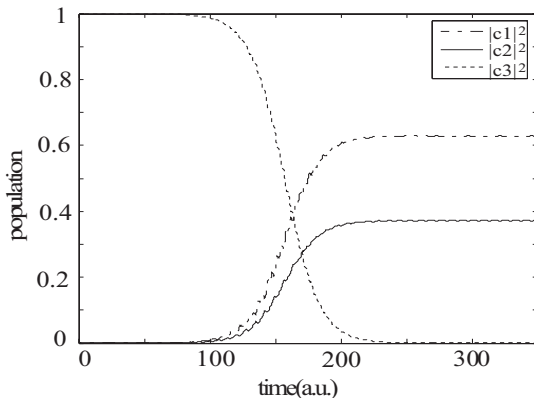


Fig. 1. Population of the control system

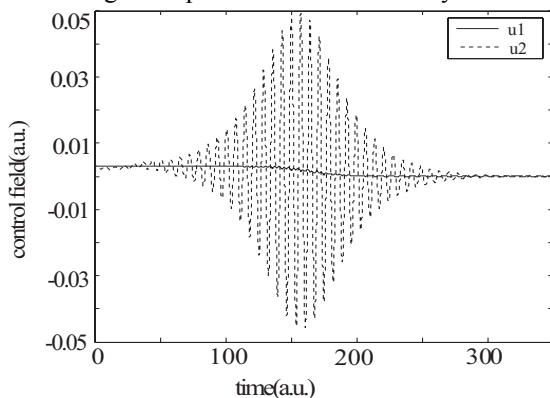


Fig. 2. Control fields

5. CONCLUSION

In this paper, the Lyapunov control based on the average value of an imaginary mechanical quantity has been proposed and proved. By using the proposed method, the quantum

Lyapunov control can complete the state transfer task from an arbitrary pure state to an arbitrary pure state for the Schrödinger equation, and from an arbitrary initial state to an arbitrary target state unitarily equivalent to the initial state for the quantum Liouville equation in most cases. The solutions of the convergence problems of quantum Lyapunov control based on the average value of an imaginary mechanical quantity establishes a completed quantum Lyapunov control theory in closed quantum systems, which has the significance of the instructing how to achieve a high successful probability in the actual quantum experimental applications.

ACKNOWLEDGEMENTS

This work was supported partly by the National Key Basic Research Program under Grant No. 2011CBA00200.

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