

Quantum Control Strategy Based on State Distance

CONG Shuang¹ KUANG Sen²

Abstract Based on Bures distance, a Lyapunov function that represents the distance between a desired state and the actual state of a quantum system is selected. Considering the cases that an initial state is and is not orthogonal to the desired state respectively, we propose a class of control strategies with state feedback that ensures the stability of the closed-loop control system. Especially, the asymptotic stability of the control system is analyzed, deduced and proved in detail. Finally, a simulation experiment on a spin-1/2 particle system is done and the relation between the system state evolution time and control value is analyzed with different parameters. Research results have general theoretical meaning for control of quantum systems.

Key words Quantum system, feedback control, Lyapunov function, stability

1 Introduction

Miniaturization of electronic circuits and devices, and the advances in laser technology make the quantum system control become an increasingly important research field. It involves control of molecular dynamics, quantum calculating, nuclear magnetic resonance (NMR), design of semiconductor nanometric devices, quantum information processing, quantum communication and so on^[1,2].

State steering of quantum systems is an important object in quantum control, *i.e.* when an initial state and a final one are given, how to look for some realizable control fields to drive the initial state to the final one. Many design methods may achieve this aim, such as optimal control technique, decoupling techniques, factorization techniques of the unitary group, and Lyapunov-based techniques. The paper is devoted to Lyapunov-based technique and theoretically designs a Lyapunov function representing the distance between the two states. According to Lyapunov stability law, one can achieve the quantum evolution from an initial state to a desired one. In comparison to [3], the main contributions of this paper include the following aspects. Firstly, the case that an initial state is orthogonal to a final state is developed. Secondly, the asymptotic stability of the system is studied in a new style. Moreover, the simulation experiment on a spin-1/2 particle system is done and the influence of different parameters on control results is obtained. Especially, the procedure for controller designing is given.

2 Selection of Lyapunov function

In physics, if all the physical quantities representing a system are given, one will know its states^[4]. The development of quantum theory shows that the wave functions of a quantum system are its states. By expanding all the states in the Hilbert space of a quantum system as the linear combination of the eigenfunctions of a mechanical quantity, one can get the same dimensional coordinate vectors. Let the dimension equal n . Evidently, the n dimensional vector space C^n is isomorphic to the Hilbert space. Correspondingly, all the quantum mechanical objects, such as quantum operators, evolution equations and so on, are described in terms of their coordinate vectors or matrixes.

Generally, the square of the error between the actual

state and the desired state of a system is usually selected as a Lyapunov function. In the paper, the distance between an actual state and a desired state is taken as a Lyapunov function. Thus the distance decreases continuously when the time derivative of the Lyapunov function is kept non-positive. There are many notions of the distance between states. However, the meaning of Bures distance is very intuitional, which represents the Euclidean distance between two equivalence classes. Therefore, Bures distance is adopted. Its definition is^[3]

$$d_B(|\psi_1\rangle, |\psi_2\rangle) = \min_{\theta} \| |\psi_1\rangle - e^{i\theta} |\psi_2\rangle \| \quad (1)$$

where $\theta \in R$, which represents an arbitrary phase. One can prove

$$d_B^2(|\psi_1\rangle, |\psi_2\rangle) = 2(1 - |\langle\psi_1|\psi_2\rangle|) \quad (2)$$

Considering inconvenience in norm calculating and conventional processing, we can choose the following function as a Lyapunov function:

$$V = \frac{1}{2} (1 - |\langle\psi_f|\psi\rangle|^2) \quad (3)$$

Comparing (2) with (3), one knows that V can represent the distance between final state $|\psi_f\rangle$ and actual state $|\psi\rangle$ at an arbitrary time. The physical meaning of (3) is evident: $|\langle\psi_f|\psi\rangle|^2$ represents the transition probability from $|\psi\rangle$ into $|\psi_f\rangle$, and when state $|\psi\rangle$ is driven entirely into state $|\psi_f\rangle$, $V = 0$, and correspondingly $d_B(|\psi_f\rangle, |\psi\rangle) = 0$.

3 Design of feedback control law

Given the following Schrödinger equation:

$$i\hbar|\dot{\psi}(t)\rangle = H|\psi(t)\rangle, \quad H = H_0 + H_c, \quad H_c = \sum_{k=1}^r H_k u_k(t) \quad (4)$$

where H_0 is the internal Hamiltonian, H_c is the interaction Hamiltonian generated by the interaction of the external controls and the system. Both H_0 and H_k are independent of time. $u_k(t)$ is a realizable, scalar, real-valued control function.

For simplicity and considering the practical requirement (*e.g.* in quantum chemistry an eigenstate of the inner Hamiltonian often need to be reached), one can assume that final state $|\psi_f\rangle$ is an eigenstate of the unperturbed system, *i.e.*,

$$H_0|\psi_f\rangle = \lambda_0|\psi_f\rangle \quad (5)$$

For $V = \frac{1}{2}(1 - \langle\psi_f|\psi\rangle\langle\psi|\psi_f\rangle)$, the first-order time

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1. Department of Automation, University of Science and Technology of China, Hefei, 230027, P. R. China 2. Department of Automation, University of Science and Technology of China, Hefei, 230027, P. R. China

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derivative of V is

$$\begin{aligned} \dot{V} &= \frac{1}{2} (-\langle \psi_f | \dot{\psi} \rangle \langle \psi | \psi_f \rangle - \langle \psi_f | \psi \rangle \langle \dot{\psi} | \psi_f \rangle) = \\ &= -\Re[\langle \psi | \psi_f \rangle \langle \psi_f | (-\frac{i}{\hbar})(H_0 + \sum_{k=1}^r H_k u_k) | \psi \rangle] = \\ &= -\frac{1}{\hbar} \sum_{k=1}^r u_k \Im[\langle \psi | \psi_f \rangle \langle \psi_f | H_k | \psi \rangle] \end{aligned} \quad (6)$$

It can be seen from (6) that the most reliable method is to let each item of the summation sign nonnegative so that $\dot{V} \leq 0$. Consequently, the function form of u_k may be of the following characteristics: $K_k f_k(x_k) x_k > 0$, where $K_k > 0$, $x_k = \Im[\langle \psi | \psi_f \rangle \langle \psi_f | H_k | \psi \rangle]$, $u_k = K_k f_k(x_k)$. Evidently, when the image of function $y_k = f_k(x_k)$ passes the origin of plane x_k - y_k monotonically and lies in quadrant I or III, the above requirement will be satisfied. At the same time, $f_k(x_k) = 0$ iff $x_k = 0$.

Analyzing (6), one can conclude that control u_k can not be used to solve the problems that an initial state is orthogonal to the final state and that final state $|\psi_f\rangle$ is an eigenstate of every H_k , ($k = 1, \dots, r$). Generally, it hardly occurs to the latter case. Even if it occurs, in principle one can solve it by adding some new controls. For the first case, a simple approach is to make a suitable measurement to change the state of the system. Then control u_k can be employed^[3]. However, this will bring an extra disturbance to the system. To solve this question, we take the following steps.

Writing complex number $\langle \psi | \psi_f \rangle$ in terms of its complex exponential number $\langle \psi | \psi_f \rangle = |\langle \psi | \psi_f \rangle| \cdot e^{i\angle\langle \psi | \psi_f \rangle}$ and substituting into (6) gives

$$\dot{V} = -\frac{1}{\hbar} \sum_{k=1}^r u_k \cdot |\langle \psi | \psi_f \rangle| \cdot \Im[e^{i\angle\langle \psi | \psi_f \rangle} \langle \psi_f | H_k | \psi \rangle] \quad (7)$$

Evidently, while the actual state $|\psi\rangle$ is not orthogonal to the desired final state $|\psi_f\rangle$ (i.e. $\langle \psi | \psi_f \rangle \neq 0$), the following u_k can also ensure $\dot{V} \leq 0$.

$$u_k = K_k f_k \left(\Im \left[e^{i\angle\langle \psi | \psi_f \rangle} \langle \psi_f | H_k | \psi \rangle \right] \right), (k = 1, \dots, r) \quad (8)$$

While the actual state $|\psi\rangle$ is orthogonal to the desired final state $|\psi_f\rangle$ (i.e. $\langle \psi | \psi_f \rangle = 0$), the angle of the complex $\langle \psi | \psi_f \rangle$ in (8) is unknown. In view of this, one can define

$$\text{If } \langle \psi | \psi_f \rangle = 0, \text{ then } \angle\langle \psi | \psi_f \rangle = 0^\circ \quad (9)$$

Thus u_k in (8) need not equal zero and $\dot{V} = 0$ in (7). It means that the actual state is turning around the final state $|\psi_f\rangle$ and while $\langle \psi | \psi_f \rangle \neq 0$ is satisfied because of the turn (the following Lemma 2 provides assurance to this condition), the case that $\dot{V} < 0$ will appear. And then the actual state will be driven towards the final state $|\psi_f\rangle$. So, (8) is selected as the final control field. Note that when $|\psi\rangle = |\psi_f\rangle$ is satisfied, $u_k = 0$ holds. It means that the control field will disappear automatically when the final state is reached.

4 Analysis and proof of stability

According to the function form of u_k , one can obtain $\dot{V} \leq 0$, so the whole system is stable in Lyapunov sense at least.

The conditions of asymptotic stability will be analyzed and proven as follows via LaSalle's invariance principle. Before analysis, two useful lemmas are given.

Lemma 1 With the control functions (8), if $\langle \psi(0) | \psi_f \rangle \neq 0$, then $\langle \psi(t) | \psi_f \rangle \neq 0, (t > 0)$ holds.

Equation (3), conditions $\dot{V} \leq 0$ and $\langle \psi(0) | \psi_f \rangle \neq 0$ may be used to prove the result.

Lemma 2 Suppose that $\langle \psi(0) | \psi_f \rangle = 0$. If $\sum_{k=1}^r (K_k \cdot f_k(\Im[\langle \psi_f | H_k | \psi(0) \rangle]) \cdot \langle \psi_f | H_k | \psi(0) \rangle) \neq 0$ is satisfied, then $\langle \psi(t) | \psi_f \rangle \neq 0, (t > 0)$ holds.

Proof. When the system runs for an infinitesimal time interval, i.e. $t = dt$, one has $|\psi(dt)\rangle \approx e^{-iHdt/\hbar} \cdot |\psi(0)\rangle \approx (1 - \frac{iH}{\hbar} dt) |\psi(0)\rangle$. Furthermore, one can prove $\langle \psi_f | \psi(dt) \rangle \neq 0 \iff \sum_{k=1}^r (u_k(dt) \cdot \langle \psi_f | H_k | \psi(0) \rangle) \neq 0$.

Here, $u_k = \lim_{dt \rightarrow 0} K_k f_k(\Im[e^{i\angle\langle \psi_f | \psi(dt) \rangle} \langle \psi_f | H_k | \psi(dt) \rangle]) = K_k f_k(\Im[\langle \psi_f | H_k | \psi(0) \rangle])$. And then according to Lemma 1, this lemma will be proved. \square

Note that the condition in Lemma 2 is easily satisfied in practice since both K_k and H_k have the degree of the freedom of selection.

LaSalle's principle says that the trajectories of the closed-loop system converge to the largest invariant set contained in $\dot{V} = 0$. So, the set of states such that $\dot{V} = 0$ need to be characterized.

Proposition 1 With the control function (8), the following three conditions are equivalent in the case that an initial state isn't orthogonal to the final state or that an initial state is orthogonal to the final state and for $t > 0$ the condition in **Lemma 2** is satisfied.

$$1) \quad \dot{V} = 0 \quad (10)$$

$$2) \quad i\hbar|\dot{\psi}\rangle = H_0|\psi\rangle \quad (11)$$

$$3) \quad \langle \psi_f | (\lambda_k I - H_k) | \psi \rangle = 0, (\lambda_k \in R, k = 1, \dots, r) \quad (12)$$

Proof. As can be seen from (8), $\dot{V} = 0 \iff |\langle \psi | \psi_f \rangle| = 0$ or $\Im[e^{i\angle\langle \psi | \psi_f \rangle} \langle \psi_f | H_k | \psi \rangle] = 0 \iff |\langle \psi | \psi_f \rangle| \cdot \Im[e^{i\angle\langle \psi | \psi_f \rangle} \langle \psi_f | H_k | \psi \rangle] = 0 \iff \Im[\langle \psi | \psi_f \rangle \langle \psi_f | H_k | \psi \rangle] = 0 \iff \lambda_k \langle \psi_f | \psi \rangle = \langle \psi_f | H_k | \psi \rangle, (\lambda_k \in R, \langle \psi | \psi_f \rangle \neq 0) \iff \langle \psi_f | (\lambda_k I - H_k) | \psi \rangle = 0, (\lambda_k \in R, k = 1, \dots, r)$. Thus, 1) \iff 3) has been proved.

1) \implies 2) is proved as follows. From the previous deducing process, condition 1) is equivalent to condition $\lambda_k \langle \psi_f | \psi \rangle = \langle \psi_f | H_k | \psi \rangle, (\lambda_k \in R, \langle \psi | \psi_f \rangle \neq 0)$. Substituting this equation into (8) gives:

$$\begin{aligned} u_k &= K_k f_k(\Im[e^{i\angle\langle \psi | \psi_f \rangle} \lambda_k \langle \psi_f | \psi \rangle]) = \\ &= K_k f_k(\lambda_k |\langle \psi_f | \psi \rangle| \Im[e^{i\angle\langle \psi | \psi_f \rangle} e^{i\angle\langle \psi_f | \psi \rangle}]) = 0 \end{aligned}$$

And then by substituting u_k into (4), one obtains $i\hbar|\dot{\psi}\rangle = H_0|\psi\rangle$.

2) \implies 1). Comparing (8) with (4), one has $\sum_{k=1}^r H_k u_k |\psi\rangle = 0 \implies \langle \psi_f | \sum_{k=1}^r H_k u_k |\psi\rangle = \sum_{k=1}^r u_k \langle \psi_f | H_k |\psi\rangle = 0 \implies \sum_{k=1}^r u_k e^{i\angle\langle \psi | \psi_f \rangle} \langle \psi_f | H_k |\psi\rangle = 0$. Since u_k is a real

scalar function, $\sum_{k=1}^r u_k \cdot |\langle \psi | \psi_f \rangle| \cdot \Im [e^{i\angle \langle \psi | \psi_f \rangle} \langle \psi_f | H_k | \psi \rangle] = 0$ holds, i. e. $\dot{V} = 0$. So, 1) \iff 2). \square

The above three conditions characterize the state set such that $\dot{V} = 0$ at some specific evolving moment. Obviously, these conditions can not explain the asymptotic stability of the system. In other words, it should be considered whether $\dot{V} = 0$ holds after the moment. From this point of view, one can find the largest invariant set of the closed-loop system.

Assume that $\dot{V}(t_0) = 0$ at time t_0 . The case that state $|\psi\rangle$ does not evolve towards target state $|\psi_f\rangle$ means that $\dot{V}(t_1) = 0$ at time $t_1 = t_0 + dt$, $\dot{V}(t_2) = 0$ at time $t_2 = t_1 + dt, \dots$. At the same time, state evolves freely starting from state $|\psi(t_0)\rangle$. By linearizing the unitary operator of the state at every time, one can obtain in turn. (setting $\hbar = 1$)

$$\begin{aligned} t_0 : \Im [\langle \psi(t_0) | \psi_f \rangle \langle \psi_f | H_k | \psi(t_0) \rangle] &= 0 \\ t_1 : \Im [\langle \psi(t_1) | \psi_f \rangle \langle \psi_f | H_k | \psi(t_1) \rangle] &= 0 \\ \iff \Im [\langle \psi(t_0) | (I + iH_0 dt) | \psi_f \rangle \langle \psi_f | H_k (I - iH_0 dt) | \psi(t_0) \rangle] \\ &\approx \Im [i \langle \psi(t_0) | \psi_f \rangle \langle \psi_f | [H_0, H_k] | \psi(t_0) \rangle] dt = 0 \\ \iff \Im [i \langle \psi(t_0) | \psi_f \rangle \langle \psi_f | [H_0, H_k] | \psi(t_0) \rangle] &= 0 \end{aligned}$$

Similarly,

$$t_2 : \Im [i^2 \langle \psi(t_0) | \psi_f \rangle \langle \psi_f | [H_0, [H_0, H_k]] | \psi(t_0) \rangle] = 0$$

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Set $[H_0^{(n)}, H_k] = \underbrace{[H_0, [H_0, \dots, [H_0, H_k]]]}_{n \text{ times}}$, the above

equations read

$$\Im [i^n \langle \psi(t_0) | \psi_f \rangle \langle \psi_f | [H_0^{(n)}, H_k] | \psi(t_0) \rangle] = 0, (n = 0, 1, 2, \dots) \quad (13)$$

In H_0 representation, H_0 is diagonal. One may let $H_0 = \text{diag}[\lambda_1, \lambda_2, \dots, \lambda_N]$ and $|\psi(t_0)\rangle = [\psi_1, \psi_2, \dots, \psi_N]^T$. Assuming H_0 is not degenerate, then N eigenstates of H_0 may be denoted as $[1, 0, \dots, 0]^T, [0, 1, \dots, 0]^T, \dots, [0, 0, \dots, 1]^T$. For convenience, one can always assume that $|\psi_f\rangle = [0, 0, \dots, 1]^T$. Then, the commutator $[H_0^{(n)}, H_k]$ reads

$$[H_0^{(n)}, H_k] = ((\lambda_i - \lambda_j)^n (H_k)_{ij}), (k = 1, \dots, r) \quad (14)$$

Substituting into (13), one has

$$\Im [i^n \psi_N^* \sum_{j=1}^N (\lambda_N - \lambda_j)^n (H_k)_{Nj} \psi_j] = 0, (k = 1, \dots, r) \quad (15)$$

In typical multiple-level systems, H_k has its diagonal entries zero. Accordingly, for $n = 0$, (13) becomes $\Im [\psi_N^* \sum_{j=1}^{N-1} (H_k)_{Nj} \psi_j] = 0$. Set

$$\xi = [(H_k)_{N1} \psi_1, (H_k)_{N2} \psi_2, \dots, (H_k)_{N, N-1} \psi_{N-1}]^T$$

$$\Lambda = \text{diag}[\lambda_N - \lambda_1, \lambda_N - \lambda_2, \dots, \lambda_N - \lambda_{N-1}]$$

$$M = \begin{bmatrix} 1 & 1 & \dots & 1 \\ (\lambda_N - \lambda_1)^2 & (\lambda_N - \lambda_2)^2 & \dots & (\lambda_N - \lambda_{N-1})^2 \\ \vdots & \vdots & \vdots & \vdots \\ (\lambda_N - \lambda_1)^{2(N-2)} & (\lambda_N - \lambda_2)^{2(N-2)} & \dots & (\lambda_N - \lambda_{N-1})^{2(N-2)} \end{bmatrix}$$

For $n = 0, 2, 4, \dots$, (13) may read $\Im (\psi_N^* M \xi) = 0$. Since M is a non-singular real matrix, this equation is equivalent to $M \Im (\psi_N^* \xi) = 0$, i.e.

$$\Im (\psi_N^* \xi) = 0 \quad (16)$$

For $n = 1, 3, 5, \dots$, (13) may read $\Re (\psi_N^* M \Lambda \xi) = 0$. Similarly, one can obtain

$$\Re (\psi_N^* \xi) = 0 \quad (17)$$

Considering (16) and (17), one has

$$\psi_N^* \xi = 0 \quad (18)$$

According to Lemmas 1 and 2, for $t_0 > 0$, $\langle \psi(t_0) | \psi_f \rangle \neq 0$, i. e. $\psi_N^* \neq 0$. Substituting into (18), one can obtain

$$\xi = 0 \quad (19)$$

Generally, (19) may read

$$\langle \psi_f | H_k | \psi(t_0) \rangle = 0, (k = 1, \dots, r) \quad (20)$$

Based on the above reasoning, we obtain the following theorem.

Theorem 1 Consider system (4) with the control field (8). If the spectrum of H_0 is not degenerate, then the largest invariant set of the closed-loop system is $S^{2N-1} \cap E$, $E = \{|\psi\rangle \mid \langle \psi_f | H_k | \psi \rangle = 0, k = 1, \dots, r\}$. If all the solutions of $\langle \psi_f | H_k | \psi \rangle = 0, (k = 1, \dots, r)$ are within the same equivalence class, then the closed-loop system will be asymptotically stable.

5 Application to a spin-1/2 particle system

There are many advantages in a spin-1/2 particle system^[5]. In order to illustrate the effectiveness of the method proposed in this paper, here the system simulation experiment will be given. Suppose that the spin-1/2 particle system is controlled only by one field and the control function $u(t)$ varies the electromagnetic field in the y direction^[6]. The spin is discussed in σ_z representation. The Schrödinger equation of the system is

$$i\hbar |\dot{\psi}(t)\rangle = (H_0 + H_1 u_1(t)) |\psi(t)\rangle$$

where $H_0 = \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$, $H_1 = \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$, setting $\hbar = 1$.

According to linear superposition principle, to perform the simplest logic NOT-gate operation (exchanging probabilities), state $|\psi\rangle$ must be driven to switch between two eigenstates $|0\rangle = [1, 0]^T$ and $|1\rangle = [0, 1]^T$. Now assume that initial state $|\psi(0)\rangle = [1, 0]^T$ and final state $|\psi_f\rangle = [0, 1]^T$. When $K_1 > 0$ in (8), the condition in Lemma 2 is satisfied. Therefore, the control field (8) is fit for this system.

For this example, one has $\langle \psi_f | H_1 | \psi \rangle = 0$, i. e. $\langle 1 | \sigma_y | \psi \rangle = 0$. This equation admits the only solution $|\psi\rangle = |1\rangle$ (without regard to the global phase). According to the Theorem 1, the system is asymptotically stable.

Setting $|\psi\rangle = [c_1, c_2]^T$ and choosing the simple sign function as the control function for the sake of easy realization, one has

$$u_1 = K_1 \text{sign}(\Im [e^{i\angle \langle \psi | \psi_f \rangle} \langle \psi_f | H_1 | \psi \rangle])$$

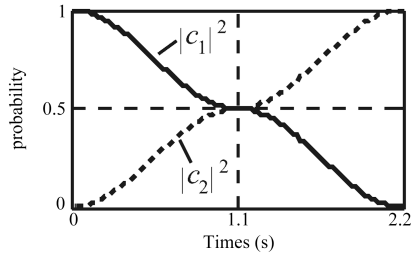


Fig. 1 Probability of the state evolution

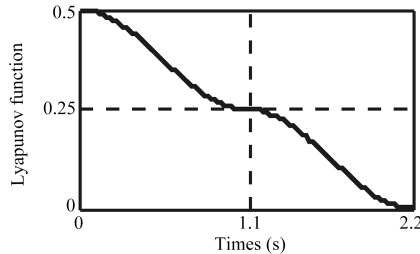


Fig. 2 Lyapunov function during the state evolution

where $K_1 > 0$. Apparently, $x \text{sign}(x) \geq 0$, the requirement for control field is satisfied. And at the same time, the control function has the form of simple bang-bang control. With $K_1 = 1$, time step length $\Delta t = 0.01 \text{sec.}$, and control time $t = 2.2 \text{sec.}$, the simulation results are shown in Figs. 1–3.

According to Fig. 1, at an arbitrary moment $|c_1|^2 + |c_2|^2 = 1$ holds, *i. e.* probability conservation. Based on Fig. 2, one can draw the conclusion: at $t_f = 2.2 \text{sec.}$, basically $V = 0$ is satisfied and state transfer is finished.

After repetitious experiments, the following rules are obtained: When parameter K_1 is fixed, t_f (time when the equivalence class of the final state is reached) does not vary with time step length Δt and decreases with parameter K_1 increasing.

6 Conclusion

By constructing the distance between an actual state and the desired state as a Lyapunov function, this paper gives the whole design process of a type of controller with state feedback of a quantum system, and deals with the problem that an initial state is orthogonal to the final state, and fully analyzes the asymptotic stability of the closed-

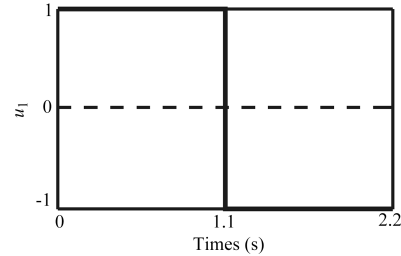


Fig. 3 Control value of the closed-loop system

loop system and gives the corresponding judgement theorem. Since the controlled state is obtained by Schrödinger equation in advance, and the control law is designed before implementing the experiment, such control strategy can be called as “program control with state feedback”.

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CONG Shuang Received her Ph.D. degree in system engineering from University of Rome “La Sapienza”, Rome, Italy, in 1995. She is currently a professor in the Department of Automation at University of Science and Technology of China. Her research interests include advanced control strategies for motion control, fuzzy logic control, neural networks control, and quantum system control. Corresponding author of this paper. E-mail: scong@ustc.edu.cn



KUANG Sen Received his master degree from Jiaozuo Institute of Technology in 2003. Now he is a Ph.D. candidate at University of Science and Technology of China. His research interests include quantum feedback control and its state estimation, and quantum optimal control. E-mail: kuangsen_ks@163.com