Quantum Control and Quantum Information Technology
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Quantum control and quantum information technology have been recognized as one of the most promising future technologies (e.g., see [1]). The development of quantum control theory is a key task for practical quantum information technology (e.g., see [2–4]). Recent advances in quantum information technologies and robust quantum information processing require the dynamics of realistic quantum systems to be characterized and controlled with unprecedented accuracy and efficiency. The interactive promotion between the two fields is a rapidly developing research area. The purpose of this special issue is to provide an account of the state of the art in this fast moving and cross-disciplinary field.

18 papers have been received for this special issue and 9 among them have been accepted for publication. The paper by C. Chen et al. presents a survey on the recent development of closed-loop control strategies in quantum control including closed-loop learning control and quantum feedback control as well as an introduction to quantum robust control. The paper by S. Cong and F. Meng presents a survey on Lyapunov control of quantum systems which is a "feedback design" and "open-loop control" strategy. The paper by S. N. Khonina et al. develops an algorithm for solving the steady-state Schrödinger equation for a class of potentials. The paper by S. Zhao et al. proposes a hybrid impulsive control method combined with Lyapunov control to achieve a more accurate convergence for a class of nonideal quantum systems. The paper by V. Tiporlini and K. Alameh investigates the principles of operation and the optimal design of an optically pumped quantum magnetometer. The paper by W. Yang and J. Sun investigates the Lyapunov control of finite-dimensional quantum systems with impulsive control fields. The paper by M. Li et al. proposes a feedback control scheme through Rabi oscillation stabilization to preserve the coherence in cavity QED. The paper by Y. Xing and J. Wu presents a quantum control method to control the Shannon entropy of quantum systems. The paper by M. Li proposes a numerical simulation algorithm for stochastic process of direct photodetection of a driven two-level system.

Acknowledgment

We appreciate all the authors who submitted their papers to the special issue. We hope that the special issue will be of interest to scientists in quantum control and quantum information technology.

Daoyi Dong
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Min Jiang
Lin-Cheng Wang

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Review Article

Closed-Loop and Robust Control of Quantum Systems

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For most practical quantum control systems, it is important and difficult to attain robustness and reliability due to unavoidable uncertainties in the system dynamics or models. Three kinds of typical approaches (e.g., closed-loop learning control, feedback control, and robust control) have been proved to be effective to solve these problems. This work presents a self-contained survey on the closed-loop and robust control of quantum systems, as well as a brief introduction to a selection of basic theories and methods in this research area, to provide interested readers with a general idea for further studies. In the area of closed-loop learning control of quantum systems, we survey and introduce such learning control methods as gradient-based methods, genetic algorithms (GA), and reinforcement learning (RL) methods from a unified point of view of exploring the quantum control landscapes. For the feedback control approach, the paper surveys three control strategies including Lyapunov control, measurement-based control, and coherent-feedback control. Then such topics in the field of quantum robust control as $H_\infty$ control, sliding mode control, quantum risk-sensitive control, and quantum ensemble control are reviewed. The paper concludes with a perspective of future research directions that are likely to attract more attention.

1. Introduction

Quantum mechanical systems model the dynamical evolution characterizing physical phenomena at atomic and molecular scales. Recent progress in theories and experiments has shown that such technologies as quantum information [1] and quantum control [2–4] have many advantages over their traditional counterparts. However, practical applications of quantum information technology are still confronted with some important technical difficulties such as the control of quantum systems in the presence of uncertainties or without explicit modeling information. Developing effective control theory and methods has been recognized as a solution to such difficulties. Some tools from classical control theory have been used to analyze and solve quantum control problems, among which we recall the most widely developed ones as follows.

Closed-Loop Learning Control. Closed-loop learning control has achieved great successes in controlling the laboratory quantum phenomena [5, 6], where the optimal open-loop control strategy is hard to design directly due to the incomplete knowledge of the system models or unexpected uncertainties.

Feedback Control. When a control is added to a quantum system, adjusting the control parameters according to instantaneous state of the system can make quantum control more pertinent and more effective, which will improve the control result with robustness and reliability. Feedback is such an effective control strategy in classical control theory as well as in quantum control theory, especially in the system with unpredictable disturbances in the evolution. During the past decades, different types of feedback control design methods have been studied for various applications [7–15].

Robust Control. In realistic environment, the quantum system is unavoidable to be subject to disturbances, uncertainties, and incomplete knowledge. These factors can all be viewed as uncertainties in the control field, in the Hamiltonian system,
in the field-coupling coefficient (e.g., the dipole moment), and so forth and might affect the control results [16]. In order to achieve robustness in control method and to develop new insights into complicated quantum plants (such as quantum networks), it is desirable to apply classical robust control theory into quantum domain. Various kinds of robust control approaches [17–23] have been proposed, especially in the communities of control science.

All of these three kinds of approaches aim at optimizing the control performances for quantum systems that have no perfect models or are subject to uncertainties. But they are different from each other regarding specific motivations, methods, and applications. A brief comparison between these three kinds of approaches is shown in Table 1, and, in the following sections, we give a self-contained survey on these promising research areas and provide interested readers with a general idea for further studies.

The remaining of the paper is organized as follows. In Section 2, the closed-loop learning control problems of quantum systems are defined with the concept of quantum control landscape, and three kinds of closed-loop learning control methods (e.g., gradient-based, GA, and RL methods) are reviewed. Section 3 introduced several feedback control approaches including Lyapunov control, measurement-based feedback control, and coherent-feedback control. Then such quantum robust control approaches as $H_\infty$ control, sliding mode control, quantum risk-sensitive control, and quantum ensemble control are surveyed in Section 4. Conclusions and the authors’ perspective on the future challenges in the associated fields are summarized in Section 5.

2. Closed-Loop Learning Control

Learning control is an effective control method that can learn from experience and optimize the system performance by searching for the best control strategy in an iterative way. When applied to the control of quantum systems, as presented in [5], the closed-loop learning control procedure generally involves three elements: (i) a trial laser control input design, (ii) the laboratory generation of the control that is applied to the sample and subsequently observed for its impact, and (iii) a learning algorithm that considers the prior experiments and suggests the form of the next control input. It is clear that, for each trial of control, it is an open-loop control, while the control performance will be sent back to the learning algorithm to direct the optimization for the optimal control strategy.

The control objective is usually formulated as an optimal control problem by converting the problem into a problem of optimizing a functional of such control parameters as the quantum states, control inputs, control time, and so on. In order to systematically study the relationship between the time-dependent controls and the associated values of the objective functional, a notion of quantum control landscape [24, 25] is defined and related theories are also well developed. In this section, we will survey the area of closed-loop learning control from the point of view of quantum control landscape and introduce several practical and promising learning methods to explore the quantum control landscape, which includes the gradient-based methods, stochastic searching methods (e.g., genetic algorithm), and reinforcement learning methods.

2.1. Quantum Control Landscape: A Unified View for Closed-Loop Learning Control. In recent years, quantum control landscapes [25] have attracted more and more attention in the research field of quantum control. A control landscape is defined as the map between the time-dependent control Hamiltonian and associated values of the control performance functional. For example, as shown in Figure 1, the performance function $J(u)$ is defined as the functional of the control strategy $u = u_i, i = 1, 2, \ldots, M$, where $M$ is a positive integer that indicates the number of the control variables ($M = 2$ for the case shown in Figure 1).

Quantum control aims to manipulate the dynamics of system evolution on the atomic and molecular scales, and most quantum control problems can be formulated as the maximization of an objective performance function. From a unified point of view, the closed-loop learning control is the approach of exploring a quantum control landscape to find the optimal control strategy where the objective function reaches its maximum or minimum. For the past decades, various algorithms have been proposed to explore the control landscapes for both theoretical studies and applications [24–29]. Most traditional learning methods can also be adopted to analyze or explore different kinds of control landscapes. In the next subsection, we survey these existing successful methods and classify them into three categories, that is, gradient-based methods, stochastic searching methods, and reinforcement learning methods.

2.2. Typical Learning Control Methods to Explore Quantum Control Landscape

2.2.1. Gradient-Based Methods. Gradient-based methods are one of the most important kinds of learning and optimization control methods for quantum systems [30, 31]. A well-developed gradient-based method called D-MORPH search algorithm is introduced in [32].

For most gradient-base methods, for example, we can introduce a time-like variable $s$ to characterize different control strategies $u^{(s)}(t)$. A gradient flow in the control space can be defined as

$$\frac{du^{(s)}(t)}{ds} = -\nabla J(u^{(s)}(t))$$

$$= - \left( \frac{\partial J}{\partial u_1(t)}, \frac{\partial J}{\partial u_2(t)}, \ldots, \frac{\partial J}{\partial u_M(t)} \right),$$

where $\nabla J(u^{(s)}(t))$ is the gradient of $J$ with respect to the control strategy $u^{(s)}(t)$.
Table 1: Closed-loop and robust control approaches for quantum systems.

<table>
<thead>
<tr>
<th></th>
<th>Motivations</th>
<th>Typical methods</th>
<th>Applications</th>
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<tbody>
<tr>
<td>Closed-loop learning control</td>
<td>Direct the control results and procedures in an iteratively learning way</td>
<td>(1) Gradient-based methods</td>
<td>Controlling laboratory quantum phenomena with incomplete knowledge or unexpected uncertainties, for example, optimal laser control design.</td>
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<td></td>
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<td>(2) Stochastic searching (GA)</td>
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<td>(3) RL methods</td>
<td></td>
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<tr>
<td>Feedback control</td>
<td>Adjust control parameters according to instantaneous feedback information</td>
<td>(1) Lyapunov control</td>
<td>Quantum state transition control, entanglement control, design of quantum gates, and so forth.</td>
</tr>
<tr>
<td></td>
<td></td>
<td>(2) Measurement-based control</td>
<td></td>
</tr>
<tr>
<td></td>
<td></td>
<td>(3) Coherent-feedback control</td>
<td></td>
</tr>
<tr>
<td>Robust control</td>
<td>Design control to achieve the best objective functional under the possible worst uncertainties</td>
<td>(1) $H^\infty$ control</td>
<td>Control design for quantum systems that are fragile and are subject to various kinds of uncertainties.</td>
</tr>
<tr>
<td></td>
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<td>(2) Sliding mode control</td>
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<td>(3) Risk-sensitive control</td>
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<td>(4) Quantum ensemble control</td>
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</table>

Choosing an arbitrary control strategy $u^0(t)$, $t \in [0, T]$, we can find the optimal one using gradient flow by solving the following initial value problem:

$$\frac{d u^{(s)}}{ds} = -\nabla J \left( u^{(s)}(t) \right),$$

(2)

$$u^{(0)}(t) = u^0(t).$$

According to (2), generally, we can approach the optimal control strategy by a forward Euler method over the $s$-domain; that is,

$$u(s + \Delta s, t) = u(s, t) - \Delta s \nabla J \left( u^{(s)}(t) \right).$$

(3)

It is clear that, for a quantum control problem, the gradient-based methods are most likely effective provided that (i) we can get the gradient easily and (ii) there are no traps on the control landscape (otherwise, the learning process may get into the traps and cannot reach the maxima). Fortunately, as argued in [5, 33], it is surprising that, under certain conditions, most of the control landscapes are trap free, and it is easy to find the optimal solution for controlling most of the quantum phenomena. But for more complex tasks, we cannot guarantee the previous conditions or the gradient is hard to acquire, and hence other global searching methods for the closed-loop learning control are necessary.

2.2.2. Stochastic Searching Methods. Most of the stochastic searching methods are global searching methods and can step over traps of local maxima. One of the most widely used methods is genetic algorithm (GA), which has also achieved great success in the closed-loop learning control of laboratory quantum systems.

In the early 1990s, Judson and Rabitz [34] use a GA learning procedure to direct the production of pulses with a laboratory measurement device. Thereafter, GA methods have been widely applied to various quantum control problems. For example, in [35], an evolutionary algorithm is applied to femtosecond pulse shaping in optimal control experiments. Tsuobuchi and Momose [36] use the GA algorithm to optimize the pulse shape for rovibrational wave-packet manipulation. Atabek et al. [37] use evolutionary algorithms for the optimal laser control of molecular orientation. The control and optimization prospects in the frequency domain are also studied theoretically using GA and shaping Fourier-limited pulses [38].

For more details about stochastic learning control methods like GA, for the laboratory closed-loop learning control, please refer to [6], where these methods are discussed within the concept of experimental adaptive feedback control (AFC).

2.2.3. Reinforcement Learning Methods. Reinforcement learning (RL) [39] is an active area of machine learning and has been extensively applied to traditional control problems ranging from operations research to robotics [40, 41]. Compared with other learning methods, RL is a learning technique based on trial and error and is a more general learning approach that can learn from experience and show great adaptability through an iterative way. That is to say, RL involves approximating solutions to stochastic optimal control problems under the condition of incomplete knowledge of the system, where the feedback for the closed loop is an imprecise value called reward or penalty. So RL methods are also suitable for control design of quantum systems [18] where it is difficult to get a good model or the searching problems are too complex to solve with computational efficiency.
On the other hand, the quantum characteristics also have inspired new algorithms for traditional RL methods. Dong et al. [42] proposed a new learning paradigm called quantum reinforcement learning (QRL) which fuses quantum computation with RL. In their study, the states \{s_i\} or actions \{a_i\} in traditional RL are denoted as the corresponding orthogonal quantum states and are called the eigen states \{\{s_i\}\} or eigen actions \{\{a_i\}\} in QRL. Here the action \(a_i\) represents the possible operation (or control) that can accomplish the state transition between two states. The state \(s_i\) can represent \(|\phi_i\rangle\) and the action \(a_i\) represents the control function that can drive \(|\phi_i\rangle\) to \(|\phi_{i+1}\rangle\). This kind of representation with a parallel updating mechanism can speed up the learning process and improve the learning performance as well. Compared with the traditional RL, the QRL algorithm learns faster, its convergence range is much larger, and the learning rate is much easier to tune. QRL has been successfully applied for incoherent control of quantum systems [18]. Other quantum-inspired RL methods have also been studied for traditional control problems [43, 44].

Due to the strong learning and adaptive abilities, RL-based methods are promising for the exploration of quantum control landscapes and can be used for those quantum control problems where gradient-based or GA methods cannot work well. Thus the gradient-based methods (local search methods), GA methods (stochastic global search methods), and RL methods (global search methods but sometimes use the direction of gradient-like rewards) constitute three typical and different searching methods to explore the quantum control landscapes.

### 3. Feedback Control of Quantum Systems

Quantum feedback control includes two central steps, that is, getting the information from the system and adding the control to the quantum system. The information of the quantum system can be obtained by two ways, precisely calculating the evolution of the system or fetching it from the quantum systems by some methods such as measurement. The former method is limited since a quantum system may have many unexpected affections during its evolution, while for the latter method, the measurement on a quantum system will unavoidably influence the states of the measured quantum system, making the situation more complex when applying feedback to quantum systems.

For a system with predictable state in the system, one can easily design the control field according to the instantaneous state of the system, and quantum Lyapunov control theory is such a kind of quantum control methods which obtain the message by exact simulation of the system. Actually, quantum Lyapunov control theory is only a feedback design of open-loop control theory, based on the artificial simulation of the system; thus it cannot be used in the case of unknown initial states or in the presence of unpredictable disturbance to the system.

There are two strategies for feedback control of quantum systems, measurement-based feedback, and coherent-feedback quantum control. The former strategy is to measure some quantum observable or signals of the system and to use and process the measurement results in a controller to produce a classical control signal that drives a suitable actuator, such as a laser beam or a potential well, which exerts direct influence on the quantum system to be controlled. The latter strategy is to use another quantum system without measurement, a full quantum controller, and connect it with the quantum system to be controlled in a feedback loop.

In the next three subsections, we will give a detailed survey of the above mentioned Lyapunov, measurement-based, and coherent quantum feedback control theories.

#### 3.1. Feedback-Designed Open-Loop Quantum Control: Lyapunov Control

Quantum Lyapunov control uses feedback design to construct control fields but applies the fields into quantum systems in an open-loop way. It has been proposed as a good candidate for quantum state transfer [45, 46] and provides us with a simple way to design control fields without measurement and feedback ([47–57]).

Lyapunov function of quantum states is the central concept in quantum Lyapunov control theory; a function \(V\) is specified to design time-varying control fields. The system with state \(\rho\) converges to the target state given by \(V\) which monotonically decreases (or increases) to its minimum (or maximum), which is an observation \(P\) of the dynamics that are closely related to some property of target states,

\[
V (\rho) = \text{Tr} (P \rho),
\]

and \(V\) just stands for the distance between the present state and the target state. Then let the derivation of the Lyapunov function \(\dot{V} < 0\), which leads to the evolution of the system to the target state.

Assume that a closed quantum system with the free Hamiltonian \(H_0\) and the time-dependent control Hamiltonian \(H_c(t)\) can be described by the following Liouville equation

\[
\frac{d\rho(t)}{dt} = -i [H_0 + H_c(t), \rho(t)].
\]

Then the time derivative of the Lyapunov function can be calculated to design the control fields. By requiring

\[
\dot{V} = \text{Tr} (-i P [H_0 + H_c(t), \rho(t)]) < 0,
\]

one can work out the requirement of the parameter of the control Hamiltonian \(H_c(t)\). Since the previous requirement may not completely determine the parameter, one can also find some further constraints to improve the control efficiency [57]. In essence, Lyapunov control uses the information of the system by simulation of the system, and it is a kind of feedback design control strategies.

This theory can be easily extended to the open quantum systems, such as the systems determined by

\[
\frac{d\rho(t)}{dt} = -i [H_0 + H_c(t), \rho(t)] + \mathcal{L} (\rho(t)),
\]

to study the control in open quantum systems.
In recent years, quantum Lyapunov control has been used to transfer quantum states \cite{45, 46}, to drive the states of open quantum system into the decoherence free subspaces \cite{53}, and to control the states in the decoherence free subspaces \cite{54}. Also, Lyapunov control can be used to control the entanglement of the quantum systems \cite{48, 52}.

### 3.2. Measurement-Based Feedback Control

Measurement-based feedback (MFC) uses the measurement results to produce a classical control signal to drive a suitable actuator which exerts direct influence on the quantum system to be controlled \cite{4}. During the MFC process, one can perform measurement on the system to get some information of the system state and then design the control law based on the estimation of the state. The system to be controlled is a quantum system, while the controller may be quantum, classical, or a quantum–classical hybrid. Different from the classical feedback control process, which can obtain the information of the system easily without disturbing it, the collapse of quantum state under the measurement process makes the problem of quantum systems rather complex.

**Markovian Quantum Feedback.** The general theory of quantum-limited feedback for continuously monitored systems was presented by Wiseman and Milburn, based on quantum measurement theory and on Hamiltonian system bath interactions \cite{11, 58}. They considered the instantaneous feedback of some measured photocurrent (homodyne detection) onto the dynamics of a quantum system, and the master equation for the resulting evolution was Markovian; that is, the measurement record is immediately fed back into the system to alter the system dynamics and may then be forgotten, while any time delay is ignored and a memoryless controller is assumed. Hence, the equation describing the resulting evolution is a Markovian master equation. This kind of feedback has already been used to reduce laser noise below the shot-noise level \cite{59} and also has been used in many aspects of physical problems, such as the control of quantum qubits \cite{60} and quantum entanglement \cite{61–64}. In case the feedback delay cannot be ignored, the feedback Hamiltonian must include a delay parameter. Time delay effect of the measurement was investigated in \cite{65}.

**Bayesian Feedback Method.** Doherty and Jacobs presented a formulation of feedback in quantum systems in which the best estimates of the dynamical variables are obtained continuously from the measurement record and fed back to control the system \cite{7, 12}. They considered some arbitrary functional of the entire history of the measurement results that can be used to alter the system evolution. The resulting equation dynamics of the system are then non-Markovian. However, the dynamics of the system and controller remain Markovian, and this is completely analogous to the situation in classical control theory. In Bayesian quantum feedback, the control process is also divided into two steps involving state estimation and feedback control. Due to the fact that, in linear systems, the estimation process may be modeled by its classical analogue, Kalman filtration and classical linear quadratic Gaussian (LQG) control theory may be applied to quantum feedback by estimation. For Bayesian quantum feedback, it uses a more general form of control Hamiltonian with more information from the measurement.

It has been compared in \cite{14} the Bayesian and Markovian feedback quantum controls, where it was proved that Bayesian feedback is never inferior, and since it uses more information, it is usually superior to Markovian feedback. However, it would be far more difficult to implement than Markovian feedback and it loses its superiority when obvious simplifying approximations are made. Thus, it is not clear which form of feedback would be better in the face of inevitable experimental imperfections. Bayesian feedback has also been used in many aspects of systems, such as the preparation of quantum states \cite{66}, and quantum error correction \cite{67, 68}.

**Weak Measurement and Nondemolition Measurement.** Making as little influence as possible during the measurement process is important to minimize disturbance to the system to be controlled. Weak measurement makes it possible to modify the evolution continuously via Hamiltonian feedback, where the Hamiltonian feedback applied to the system depends on the measurement record \cite{69}, and it can also be modeled by a stochastic master equation by introducing an ancilla system weakly coupled to the system of interest. Weak measurements and local feedback can be used to control the generation of entanglement between two qubits \cite{70}. Motivated by the proposal of Braunčzyk et al. \cite{71}, experimentally exploring the use of weak measurement \cite{72} in feedback control on a photonic polarization qubit is given in \cite{73}, as well as in the control of nonlinear quantum systems \cite{74}. Quantum nondemolition measurement preserves the integrity of the system and the value of the measured observable, which is best thought of as the ideal quantum projective measurement. Nevertheless, nondemolition does not mean that the state of the system has no wave collapse, and it is extremely difficult to carry out experimentally \cite{75}.

Although measurement-based feedback control is effective in many quantum control systems, its drawbacks are also evident. Firstly, measuring a quantum system almost inevitably disturbs it. Even a nondemolition measurement that leaves the system in the state in which it was measured still typically alters the states of the system prior to the measurement \cite{76, 77}. After fluorescence determines whether the ion is in its ground state or excited state, the initial quantum coherence between those states is irrevocably lost. Secondly, the information from the measurement is stochastic because a result of the measurement of the system jumps to one state or another probabilistically. Although the ability to apply coherent operations conditioned on the results of measurements allows the controller to compensate for the probabilistic nature of their results, the introduction of stochastic effects significantly complicates the control process. Furthermore, the measurement-based feedback is limited by its information processing speed that has to be kept up with the evolution of the system dynamics, and it cannot be used in most solid state systems whose time scales range from picoseconds to nanoseconds.
3.3. Coherent-Feedback Control. Coherent-feedback quantum control uses another quantum system as a full quantum controller and connects it with the quantum system to be controlled in a feedback loop; that is, the feedback controller itself is a quantum system, and the control operations consist of unitary transformations. This is greatly different from Markovian and Bayesian quantum feedback controls where the feedback information from measurement results is classical information and the feedback controller is a classical controller.

Since this control uses full quantum information of the system, it can perform a number of tasks that controllers using a classical information feedback loop cannot; [15]. Compared with the measurement-based feedback control, coherent-feedback control does not involve measurement, avoiding the introduction of excess measurement noise, while the controller and the system plant can be both quantum systems and are coherently connected. By coherent-feedback control, one can use coherent feedback to guide a quantum system from an unknown initial state to a desired final state without destroying the initial state. In addition, a controller can use a quantum feedback loop to drive a quantum system to a target state that is entangled with another quantum system, while entanglement is a nonlocal quantum phenomenon that cannot be created by controllers using classical feedback loops.

The very successful noise-reducing controllers, the $H^\infty$ and the linear quadratic Gaussian (LQG) controllers, have natural coherence control analogues [17, 78, 79]. By basic principles of linear quantum stochastic control theory, it has been presented that optimal and robust design of quantum coherent-feedback loops can be accomplished using sophisticated methods of system engineering [17], and an experimental implementation of coherent-feedback quantum control with optical resonators as the dynamical systems and laser beams as the coherent disturbance and feedback signals has been presented [80]. The experiments of coherent-feedback control in optical field squeezing are proposed in [81], and it was also applied to many other interesting problems, such as cooling quantum oscillator [82], spontaneous switching suppression [83], multipartite quantum entanglement generation [84], and producing optical quantum gates in a four-wave mixing process [85].

Traditional coherence feedback control was established for the Markovian environment. Recently, the non-Markovian coherence feedback control was presented [86]. However, in coherence feedback control, the controller itself will cause quantum decoherence to the controlled system even though it coherently entangles with the system [87]; thus, whether the coherent feedback is better than the open-loop control for quantum control systems needs to be investigated in depth [88].

4. Robust Control

A general formalism of quantum robust optimal control problem was given in [16], which pointed out that to design a control field that achieves the best objective functional under possible worst uncertainties is in essence a minimax problem. Reference [16] also provided a method to calculate the worst possible disturbance to the control process and to design a corresponding robust optimal control field. Another noticeable early attempt to apply robust control theory in quantum field is [89], where the small gain theorem was extended to analyze the stability of quantum feedback networks. Later, different robust control tools were systematically introduced into the quantum domain, which formulated the early development of quantum robust control.

4.1. $H^\infty$ Control of Quantum Systems. For several typical classes of noncommutative linear stochastic systems with many interesting examples in quantum technology, $H^\infty$ control theory was introduced to obtain robust controllers and developed for diverse situations and requirements.

Take the class of linear noncommutative stochastic systems in [17] for example, which encompasses some quantum and classical systems:

\[
\begin{align*}
    dx(t) &= Ax(t)dt + Bd\omega(t), \quad x(0) = x_0, \\
    dy(t) &= Cx(t)dt + Dd\omega(t),
\end{align*}
\]

where $A, B, C, D$ are, respectively, real $R_{n\times n}$, $R^{n_\omega \times n}$, $R^{m\times n_\omega}$, and $R^{n_\omega \times n}$ matrices with $n, n_\omega, m$ all positive integers and $x(t) = [x_1(t), \ldots, x_n(t)]^T$ is a vector of self-adjoint possibly noncommutative system variables, whose initial value $x_0$ consists of operators satisfying the commutation relations

\[
[x_j(0), x_k(0)] = 2i\Theta_{jk}, \quad j, k = 1, \ldots, n,
\]

where $[A, B] = AB - BA$ is the commutation operator, $\Theta_{jk}$ are components of the real antisymmetric matrix $\Theta$, and $i$ is the imaginary unit. $x_0$ is also assumed to be Gaussian with density operator $\rho$. The vector quantity $\omega$ describes the input signals and is assumed to have the decomposition

\[
d\omega(t) = \beta_\omega(t) dt + d\tilde{\omega}(t),
\]

where $\beta_\omega(t)$ is a self-adjoint, adapted process (see [90, 91]). The noise part of $\omega(t)$ is $d\tilde{\omega}(t)$, a vector of self-adjoint quantum noises with Itô table

\[
d\tilde{\omega}(t)d\tilde{\omega}^T(t) = F_\omega dt,
\]

where $F_\omega$ is a nonnegative Hermitian matrix (see [91, 92]). For more detailed description and assumptions and the physical realisability of this class of systems, one can refer to [17].

The $H^\infty$ controller synthesis problem for the class of systems described by (8)–(11) was first formulated and solved in [17]. Furthermore, this quantum $H^\infty$ control problem was extended to a time-varying version, and the corresponding solution was obtained by a dynamic game approach in [93]. For the same plant, the finite horizon dynamic game theory approach was applied in [94], and the solving process was proved equivalent to solving a corresponding deterministic continuous-time problem with imperfect state information.
The finite horizon $H^\infty$ control problem in [94] was then extended to the case of delayed measurements in [95].

To simplify the deduction process and obtain more profound results, a more special class of linear quantum systems was considered in [79], which proposed a robust controller designing method probably more easy to implement experimentally.

### 4.2. Sliding Mode Control of Quantum Systems

Sliding mode control (SMC) approach is a useful robust control tool in classical control theory and industrial applications, especially for nonlinear systems. Since many quantum systems evolve with nonlinear equations, SMC is therefore supposed to be capable of controlling some quantum phenomena [96, 97].

Reference [98] applied the SMC control method into quantum systems. Similar to the classical theory, quantum sliding mode is a system state where the system has some desirable features, such as robustness to a class of uncertainties, and features brought by eigenstates, features brought by invariant state subspaces. Once the sliding mode is selected, one needs to design control laws that can drive the system onto its sliding mode and keep the system on it, which were designed in detail by combining unitary control and periodic projective measurements in [98].

In [99], a sliding mode design method for two-level quantum systems with bounded uncertainties was proposed. The uncertainties were assumed to take the form of perturbations in the Hamiltonian, and the controller design method used the Lyapunov methodology and periodic projective measurements. These results were extended in [100], where the effect of uncertainties in driving the system state back to the sliding mode domain from outside was considered, and the measurement periods were modified when considering uncertainties described as perturbations in the free Hamiltonian. In [101], a sampled-data design approach for decoherence control of a single qubit with operator errors was proposed using a sliding mode domain concept as the required control performance.

Though sliding mode control approach was introduced into quantum systems, the appropriate combination of the essential characters of these two focuses is still worth digging. Furthermore, one may consider extending sliding mode control to open quantum systems and applying other branches of classical nonlinear control theories into the quantum domain.

### 4.3. Quantum Risk-Sensitive Control

As a modification of the common integral form of criterion, or the so-called a risk-neutral criterion, a risk-sensitive criterion takes the form of an exponential function, which results in the close connections between robust control and risk-sensitive control [102–104]. For example, risk-sensitive control is anticipated to be useful in designing robust controllers [105]. Reference [106] formulated a risk-sensitive optimal control problem for quantum systems, obtained a solution using dynamic programming, and briefly discussed the robustness properties of the risk-sensitive controllers. Reference [107] considered a risk-sensitive optimal control problem for continuously monitored open quantum systems within the framework of quantum Langevin equations and solved the problem with quantum stochastic calculus and dynamic programming. Reference [105] collected related research and systematically illustrated a quantum risk-sensitive control problem and the corresponding dynamic-programming solution. At the end of [105], the author proposed several developing directions for quantum risk-sensitive control, which include theoretical development, practical applications in quantum field, and the exploration of robustness properties.

Filtering aims to extract information from noisy signals and is inherently connected with robust control, which therefore forms robust estimation. Guaranteed-cost filtering and risk-sensitive filtering are two branches of robust estimation, which are quite promising to be extended into quantum theory. Reference [108] obtained a quantum version of the guaranteed-cost filter and showed its unique robustness character compared with optimal Kalman filter and risk-sensitive observer. Reference [23] studied a quantum risk-sensitive estimation problem and analyzed robustness properties of the filter under a discrete approximation model of the aimed quantum system. More systematic work within the associated topics remains to be done.

### 4.4. Quantum Ensemble Control

Ensemble control means controlling a continuum of dynamical systems with different values of parameters characterizing the system dynamics by using the same control signal. Ensemble control derives from the manipulation of an ensemble of nuclear spins in nuclear magnetic resonance (NMR) spectroscopy and imaging (MRI), where one often needs to develop external excitations that can simultaneously steer the ensemble of systems with variations in their internal parameters from a fiducial state to a target state [109]. Here we view the difference in parameters as system uncertainties. Hence, ensemble control forms a new systematic branch of robust control.

A fundamental question in quantum ensemble control is controllability, which determines whether the control function that transfers the system from initial states to desired target states can exist. Reference [110] introduced the notion of simultaneous controllability; that is, all individuals in the system are simultaneously controllable, and generalized controllability criteria for decomposable systems. References [111, 112] formally proposed the definition of ensemble controllability for quantum systems described by Bloch equations depending continuously on a finite number of scalar parameters and with a finite number of control inputs and analyzed ensemble controllability and optimal control of linear time-invariant systems. Ensemble controllability concerns finding open-loop controls to compensate for the dispersion in element parameters. Reference [113] cast the design of control pulses as an optimal ensemble control problem and introduced a multidimensional pseudospectrum-based solution, whose convergence was shown in [114]. Reference [115] studied the controllability of an ensemble of general finite-dimensional time-varying linear systems and gave necessary and sufficient conditions, which is in connection with singular values of the operator characterizing the system dynamics.
Reference [116] introduced a universal numerical method based on the singular value decomposition to approximate optimal ensemble control problems.

Furthermore, since ensemble is originally a notion in quantum statistics, one may anticipate introducing tools and methods in quantum statistical mechanics into quantum ensemble control to give new in sights and approaches.

5. Conclusions and Discussions

Manipulating system dynamics at the quantum scale is full of challenges for both theoretical and laboratory researchers. Closed-loop and robust control approaches are of most importance to deal with uncertainties and incomplete knowledge about the system dynamics or unexpected disturbances. To conclude this paper, we briefly discuss some open problems and promising research directions as follows.

Learning skills is very important for the control design of quantum systems where no good solutions can be easily obtained from a specific model. Although the closed-loop learning control approach for controlling quantum phenomena has been well developed since the early 1990s, more effective learning theories and algorithms need to be further explored. The experts from different fields such as quantum physics, chemical physics, control theory, computer science, and artificial intelligence need to cooperate on this exciting research area.

Feedback control is one of the most important control strategies for traditional control problems. Almost all the practical industrial control systems use feedback controllers such as PID controllers. In the feedback control approach, the deviations between the measured variable and a set point are fed back to the controller to generate appropriate control actions. When we apply feedback control methods for the quantum control systems, two problems are unavoidable, that is, the problems of measurement and time scale. Quantum state measurement is difficult and much more complex than its counterpart of traditional control systems. Time scale is another nontrivial issue for the control of quantum systems since the feedback signals are always lagging. The feedback control design needs to incorporate the time delay of the feedback signal and satisfy the time scale of the controlled quantum systems.

For practical applications, robustness is an important aspect for the design of controllers, especially for quantum systems that are subject to various kinds of uncertainties and are more fragile. The existing results mainly focus on certain kinds of quantum systems with specific models, and experiments temporarily fall behind the development of theory. In the future, more general and systematic approaches of robust control need to be developed for more general kinds of uncertainties which exist in practical applications.

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References


Research Article

Calculating the Energy Spectrum of Complex Low-Dimensional Heterostructures in the Electric Field

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An algorithm for solving the steady-state Schrödinger equation for a complex piecewise-constant potential in the presence of the electric field is developed and implemented. The algorithm is based on the consecutive matching of solutions given by the Airy functions at the band boundaries with the matrix rank increasing by no more than two orders, which enables the characteristic solution to be obtained in the convenient form for search of the roots. The algorithm developed allows valid solutions to be obtained for the electric field magnitudes larger than the ground-state energy level, that is, when the perturbation method is not suitable.

1. Introduction

The research aimed at developing high-performance computing systems, communication, and information processing means has led to the emergence of a new approach to designing the electronics components [1–6]. Within such an approach, the information is carried by the amplitude of the electron wave function in a given region of the quantum system. By applying an external $E$-field that introduces changes in the energy spectrum one can induce a controlled redistribution of the system electron density, which corresponds to the data conversion by a predetermined law.

The devices for controlled electron density redistribution can be physically implemented using structures composed of an array of tunnel-coupled quantum wells.

In a multiwell quantum structure the wave function amplitude distribution is actually determined by the interference of quantum states of different quantum wells [7]. Because of this, the electron density redistribution under the action of the external $E$-field may appear as a complex, nonmonotonic process. Then, changes in the system’s physical characteristics will also be nonmonotonic, thus opening wide opportunities for designing novel quantum devices [8].

When designing an electronic device, one needs to learn in which way the energy spectrum of the electric charge can be varied in a desired manner by exposing it to various external actions. The most popular controlling technique is by use of the electric field. In such a system, the energy spectrum can be calculated using the steady-state Schrödinger equation characterized by a designed potential structure and the constant electric field applied.

For the potential described by a piecewise-constant function, the problem can be solved by representing the wave functions as a superposition of the Airy functions. While simple heterostructures described by one or two potential energy levels enable an analytical solution to be derived, for the complex-shaped potentials the problem becomes very computationally challenging [7]. As a rule, the problem is tackled using the perturbation method [9, 10], which is only suited when the $E$-field applied is low enough.

Thus, the problem of development and implementation of a numerical method for calculating the energy spectrum of a complex-shaped potential exposed to the electric field remains relevant.

We describe an algorithm for solving the corresponding steady-state Schrödinger equation. The algorithm is based on consecutively matching the solutions at the zone boundaries with the matrix rank increasing by no more than two orders, thus allowing the procedure for seeking the characteristic equation roots to be easily implemented.

The comparison of the algorithm with the perturbation method is conducted.
2. An Algorithm for Solving Schrödinger Equation Using the Consecutive Joining

Let there be a 1D heterostructure composed of an array of homogeneous semiconductor layers (the layer boundaries being perpendicular to the Ox-axis) exposed to the E-field. If the E-field of strength F is parallel to the x-axis, the potential energy is given by

\[ U(x) = qFx + U_p, \]

where \( q \) is the absolute magnitude of the electron charge, \( U_p \) is the value of the piecewise-constant potential on the segment \( x \in [x_{p-1}, x_p] \), and \( x_p \) are the layer boundary coordinates.

Then, the Schrödinger equation takes the form

\[ -\frac{\hbar^2}{2m_p} \frac{d^2 \psi(x)}{dx^2} + (qFx + U_p) \psi(x) = E \psi(x), \]

where \( m_p \) is the effective mass and \( \psi(x) \) is the particle’s wave function.

Denote that

\[ u = b_p^{1/3} (x - c_p), \]

where \( c_p = (E - U_p)/qF \), \( b_p = (2m_p qF/\hbar^2) \).

In this case, the wave function of the argument \( u \) satisfies the Airy equation:

\[ \left\{ \frac{d^2}{du^2} - u \right\} \psi(u) = 0. \]

On each interval, the solution of (4) takes the form [11,12]

\[ \psi_p(u_p(x)) = A_p Ai(u_p(x)) + B_p Bi(u_p(x)), \]

where \( u_p(x) = b_p^{1/3}(x - c_p), x \in [x_{p-1}, x_p] \); \( Ai(x), Bi(x) \) are the Airy functions of the first and second kind, respectively.

By imposing the matching conditions of the wave functions and derivatives thereof divided by the mass on the interval (layer) boundaries, the coefficients of the solution in (5) can be represented as

\[ A_p Ai(u_{p,p}) + B_p Bi(u_{p,p}) = A_{p+1} Ai(u_{p+1,p}) + B_{p+1} Bi(u_{p+1,p}), \]

\[ \frac{1}{m_p} \left[ A_p Ai'(u_{p,p}) + B_p Bi'(u_{p,p}) \right] = \frac{1}{m_{p+1}} \left[ A_{p+1} Ai'(u_{p+1,p}) + B_{p+1} Bi'(u_{p+1,p}) \right], \]

where \( u_{p,p} = b_p^{1/3}(x_p - c_p) \).

Note that the allowed values of energy \( E \) implicitly enter in (6) in the form of the Airy function arguments in (5). In the following, we consider obtaining the characteristic equation (for \( E \)) by a simple example of an infinite quantum well and a general-form quantum well potential.

3. Infinite Triangular Potential Well

By way of illustration, the model of a triangular infinite potential well is utilized when describing the surface quantization. The potential of the infinite triangular well is described by the relation (Figure 1)

\[ U(x) = \begin{cases} \infty, & x \in [-\infty, x_0], \\ U_0 + qFx, & x \in [x_0, \infty]. \end{cases} \]

The boundary conditions define that the wave function in (5) has the zero value at the left boundary of the well (when \( x = x_0 \) and \( x \to \infty \)). Whence it follows that \( B_0 = 0 \), and thus,

\[ \psi_0(u(x_0)) = A_0 Ai(u(x_0)) = 0, \]

where \( u(x_0) = x_0 - (E - U_0)/qF(2m_0 qF/\hbar^2)^{1/3} \).

The constant \( A_0 \) in (8) is normalized on the assumption that the integral of the wave function’s squared modulus is equal to unity.

The condition in (8) holds when \( u(x_0) = a_n \), where \( a_n \) are the Airy function roots. Thus, the allowed energy values are

\[ E_n = \left[ x_0 - a_n \cdot \left( \frac{2m_0 qF}{\hbar^2} \right)^{-1/3} \right] qF + U_0. \]

Putting \( x_0 = 0 \) and using the approximate values of the Airy function roots [11,12]

\[ a_n \approx -\left[ \frac{3\pi}{8} (4n - 1) \right]^{2/3}, \]

we obtain an approximate estimate of the energy spectrum of the infinite triangular well in the explicit form (with regard to the electron charge)

\[ E_n \approx \frac{\hbar^2}{2m_0} \left[ \frac{3}{2} qF \pi (n - 0.25) \right]^{2/3} + U_0. \]

In the following, we conduct the comparison of the energy spectra of a finite-width square well with and without the E-field applied.

![Figure 1: The energy spectrum of an infinite triangular potential well.](image-url)
### 4. Infinite Square Potential Well

For a quantum well of width $2L$, the potential is (Figure 2)

$$U(x) = \begin{cases} 
\infty, & x \in [-\infty, -L], \\
U_0 + qFx, & x \in [-L, L], \\
\infty, & x \in [L, \infty].
\end{cases}$$

(12)

For a classical infinite square quantum well of width $2L$, the solution is known to take the form

$$\psi_n(x) = \sin(\alpha_n (x + L)),$$

(13)

where

$$\alpha_n = \sqrt{\frac{2m_0}{\hbar^2} (E_n - U_0)}, \quad E_n = \left(\frac{\pi n}{2L}\right)^2 \frac{\hbar^2}{2m_0} + U_0.$$  

(14)

When applying a low-value $E$-field, an approximate solution can be derived using the perturbation method [9, 10].

#### 4.1. Solving the Schrödinger Equation by the Perturbation Method

Let us consider the perturbation theory for a nondegenerate state. The steady-state Schrödinger equation (2) can be written as

$$H \left[\psi_n(x)\right] = E_n \psi_n(x),$$

(15)

where the operator $H$ takes the form

$$H = H_0 + W,$$

(16)

$W$ is the perturbation operator and $H_0$ is the nonperturbed operator whose eigenfunctions and eigenvalues are defined by (13) and (14):

$$H_0 \left[\psi_n(x)\right] = E_n^0 \psi_n(x).$$

(17)

The sought-for eigenfunction of the perturbed operator can be decomposed in terms of the unperturbed operator as

$$\psi_n(x) = \sum_{m} c_m^n \psi_m(x).$$

(18)

Substituting (18) into (15) yields

$$\sum_{m} c_m^n W \left[\psi_m(x)\right] = \sum_{m} c_m^n (E_n - E_m^0) \psi_m(x).$$

(19)

Taking the scalar product of (19) by $\psi_l^*(x)$ and with regard to the orthogonality, we obtain

$$\sum_{m} c_m^n \int \psi_l^* (x) W \left[\psi_m(x)\right] dx = c_l^n \left( E_n - E_l^0 \right),$$

(20)

$$l = 1, 2, 3, \ldots.$$

Assuming that the perturbation operator is infinitesimal, we find the energy levels and wave functions of the perturbed and unperturbed operators to be close to each other. The sought-for solution will include the second-order corrections:

$$E_n^0 \approx E_n^0 + E_n^1 + E_n^2,$$

$$\phi_n(x) = \psi_n(x) + \sum_{m \neq n} c_{m,1} \psi_m(x) + \sum_{m \neq n} c_{m,2} \psi_m(x).$$

(21)

From (20) and (21), the corrections are described by the following equations [9, 10]:

$$E_n^1 = \int \psi^*_n (x) W [\psi_n (x)] dx,$$

$$E_n^2 = \sum_{m \neq n} c_{m,1} \int \psi^*_n (x) W [\psi_m (x)] dx,$$

$$c_{m,1} = \frac{\int \psi^*_m (x) W [\psi_n (x)] dx}{(E_n^0 - E_m^0)},$$

$$c_{m,2} = \left\{ \sum_{l} c_{l,1} \int \psi^*_l (x) W [\psi_l (x)] dx - c_{n,1} \right\} \times (E_n^0 - E_m^0)^{-1}. $$

(22)

#### 4.2. Perturbations Method for an Infinite Square Potential Well in the Electric Field

In the case in question,

$$H_0 = -\frac{\hbar^2}{2m_0} \frac{d^2}{dx^2} + U_0,$$

$$W = qFx.$$

The unperturbed solutions are considered to be given by (13) and (14). In this case, the energy values for (2) are derived from the relation:

$$E_n \approx \left(\frac{\pi n}{2L}\right)^2 \frac{\hbar^2}{2m_0} + U_0 + E_n^1 + E_n^2.$$  

(24)
where
\[ E_n^1 = qF \int_{-L}^{L} \sin^2 (\alpha_n (x + L)) \, dx = qFL, \]
\[ E_n^2 = qF \sum_{m} c_{n}^{m,1} \int_{-L}^{L} \sin (\alpha_n (x + L)) \sin (\alpha_m (x + L)) \, dx - c_{n}^{m,1} E_n, \]
(25) Then, the wave functions are determined as follows:
\[ \psi_n (x) = \sin \left( (x + L) \sqrt{\frac{2m_e}{\hbar^2} (E_n - U_0)} \right) + \sum_{m \neq n} c_{n}^{m,1} \psi_m (x) + \sum_{m \neq n} c_{n}^{m,2} \psi_m (x), \]
(26) where
\[ c_{n}^{m,1} = \frac{qF \int_{-L}^{L} \sin (\alpha_n (x + L)) \sin (\alpha_m (x + L)) \, dx}{(E_n^0 - E_m^0)} , \]
\[ c_{n}^{m,2} = \left\{ qF \sum_{l} c_{n}^{l,1} \int_{-L}^{L} \sin (\alpha_n (x + L)) \sin (\alpha_l (x + L)) \, dx - c_{n}^{l,1} E_n \right\} \times \left( E_n^0 - E_m^0 \right)^{-1}. \]
(27) For the first-order approximation, all allowed energy levels in the infinite well are shifted by the same value \( qFL \), whereas for the second-order approximation the gap between the quantum well bottom and the ground state will decrease as the square of the \( E \)-field strength.

The perturbation method remains suitable until the maximal change of potential at the well boundary due to the \( E \)-field reaches the order of the ground state energy. If the \( E \)-field applied becomes larger, the direct matching algorithm described in Section 1 needs to be used.

4.3. The Matching Method for an Infinite Potential Well in the \( E \)-Field. The boundary conditions are derived on the assumption that the wave function of (5) has a zero value at the well boundaries:
\[ \psi_0 (u_{-L}) = A_0 Ai (u_{-L}) + B_0 Bi (u_{-L}) = 0, \]
\[ \psi_0 (u_L) = A_0 Ai (u_L) + B_0 Bi (u_L) = 0, \]
(28) where
\[ u_{-L} = \left( -L - \frac{E - U_0}{qF} \left( \frac{2m_e qF}{\hbar^2} \right) \right)^{1/3}, \]
\[ u_L = \left( L - \frac{E - U_0}{qF} \left( \frac{2m_e qF}{\hbar^2} \right) \right)^{1/3}. \]
(29) Thus, we obtain a homogeneous equation
\[ \begin{pmatrix} Ai (u_{-L}) & Bi (u_{-L}) \\ Ai (u_L) & Bi (u_L) \end{pmatrix} \begin{pmatrix} A_0 \\ B_0 \end{pmatrix} = 0, \]
(30) which has a nontrivial solution if the determinant is equal to zero:
\[ Ai (u_{-L}) Bi (u_L) - Ai (u_L) Bi (u_{-L}) = 0. \]
(31) This equation determines the eigenvalues \( E_n \).

The coefficient \( B_0 \) can be expressed through \( A_0 \) using one of the equations in (28):
\[ B_0 = -A_0^2 \frac{Ai (u_{-L})}{Bi (u_{-L})} = -A_0 \frac{Ai (u_L)}{Bi (u_L)}, \]
(32) with the value of the coefficient \( A_0 \) derived from the wavefunction normalization condition.

In the following, we conduct the comparison of the solutions derived by the two methods.

4.4. Comparison of the Results Derived by the Two Methods. The parameters used in the calculations are as follows: \( m_0 = 0, 1 m_e, m_e = 9.10938188 \times 10^{-31} \) kg is the electron mass, \( h = 1.054571726(47) \times 10^{-34} \) \( \) \( \) is the Planck constant, and the potential \( U \) and energy \( E \) are in electron-volts (1 eV = 1.602176487(40) \( \times 10^{-19} \) J), with the \( E \)-field given in the reduced values. In the case of interest, \( U_0 = 0 \) and the well width is \( 2L = 2 \) nm.

Table 1 gives the values of the first three allowed energy states for an infinite square well in the absent \( E \)-field, in the weak \( E \)-field and in the “strong” \( E \)-field (i.e., when the \( E \)-field strength is higher than the ground state energy).

Table 1 suggests that when applied for a strong \( E \)-field, the perturbations method produces invalid results. The matching method leads to widened band gaps between the energy states as the \( E \)-field applied is increasing. Note that applying the strong \( E \)-field results in the narrowed gap between the well bottom and the ground state energy.

Figure 3 shows the first three wave functions in the absence of the \( E \)-field, in the weak \( E \)-field and in the strong \( E \)-field derived using the matching method. According to Figure 3, with increasing \( E \)-field, the probability of the electron to be found in the potential well ceases to be symmetric, being shifted toward one of the well boundaries.

5. Infinite Square Well with a General-Form Piecewise-Linear Potential

In the general case, the potential of an infinite well in the \( E \)-field is described as
\[ U (x) = \begin{cases} \infty, & x \in [-\infty, -L], \\ U_0 + qFx, & x \in [-L, x_0], \\ \vdots \\ U_N + qFx, & x \in [x_{N-1}, x_p], \\ \infty, & x \in [x_p, L], \end{cases} \]
(33)
The last-band (-layer) coefficients can be expressed through $A_0$ and $B_0$ as
\[
\begin{pmatrix} A_N \\ B_N \end{pmatrix} = Q_{N-1} Q_{N-2} \cdots Q_1 \begin{pmatrix} A_0 \\ B_0 \end{pmatrix},
\]
(36)
where
\[
Q_p = \begin{bmatrix} Ai\left(u_{p+1}\right) & Bi\left(u_{p+1}\right) \\ \dfrac{Ai'\left(u_{p+1}\right)}{m_{p+1}} & \dfrac{Bi'\left(u_{p+1}\right)}{m_{p+1}} \end{bmatrix}^{-1} \times \begin{bmatrix} Ai\left(u_p\right) & Bi\left(u_p\right) \\ \dfrac{Ai'\left(u_p\right)}{m_p} & \dfrac{Bi'\left(u_p\right)}{m_p} \end{bmatrix}.
\]
(37)
Thus, for the coefficients $A_0$, $B_0$, $A_N$, and $B_N$ we have derived four equations in (34), (36), which form a homogeneous linear system. Putting the system's determinant equal...
to zero, we obtain a characteristic equation for deriving the eigenvalues of $E$.

Applying the algorithm of (34)–(37) for the consecutive matching of solutions at the band boundaries with use of the second-rank matrix, the characteristic equation can be put in a more convenient form.

The numerical implementation of the algorithm (34)–(37) allows a simple solution of the steady-state Schrödinger equation (2) with the complex potential of (33) to be derived. However, this calls for the use of the “exponential arithmetic” (arithmetic over numbers represented as $a \exp(b)$, where $a$ and $b$ are the number parameters). Otherwise, the software implementation will be incorrect at small values of the $E$-field: $qF < 0.5$.

Figure 4 depicts a complex-form potential with and without the $E$-field applied. Table 2 gives the corresponding values of the energy spectrum for the said potential. The wave functions distributions are shown in Figure 5.

The computation results suggest that by varying the potential form and the external $E$-field both the energy spectrum and the distribution of the probability of finding the particle in a definite heterostructure region can be essentially varied.

6. Conclusions

We have developed and implemented an algorithm for solving the steady-state Schrödinger equation for a complex piecewise-constant potential in the presence of the $E$-field. The algorithm is based on the consecutive matching of solutions given by the Airy functions at the band boundaries with the matrix rank not exceeding two, thus allowing the characteristic equation to be derived in the convenient form for the search of the roots.

It has been numerically shown that the algorithm developed allows valid solutions to be derived when the value
Table 2: Energy spectrum (first 9 values) for a complex relief.

<table>
<thead>
<tr>
<th>$E_n$</th>
<th>Zero $E$-field</th>
<th>$E^-$-field $qF = 0.1$</th>
<th>$E^-$-field $qF = 1$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$E_n$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>0.305344</td>
<td>0.493440</td>
<td>0.779213</td>
<td></td>
</tr>
<tr>
<td>0.660222</td>
<td>0.833417</td>
<td>0.338370</td>
<td></td>
</tr>
<tr>
<td>1.210436</td>
<td>1.425745</td>
<td>0.357965</td>
<td></td>
</tr>
<tr>
<td>1.492179</td>
<td>1.979392</td>
<td>0.942955</td>
<td></td>
</tr>
</tbody>
</table>

of the $E$-field applied is larger than the ground-state energy level, that is, under the conditions when the perturbation method is inapplicable.

The computation results obtained for the complex potential distribution have shown that by varying the potential profile and the value of the $E$-field applied it becomes possible to essentially vary the energy spectrum and the probability of finding the particle in one or another region of the heterostructure.

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Research Article

Controlling the Shannon Entropy of Quantum Systems

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This paper proposes a new quantum control method which controls the Shannon entropy of quantum systems. For both discrete and continuous entropies, controller design methods are proposed based on probability density function control, which can drive the quantum state to any target state. To drive the entropy to any target at any prespecified time, another discretization method is proposed for the discrete entropy case, and the conditions under which the entropy can be increased or decreased are discussed. Simulations are done on both two- and three-dimensional quantum systems, where division and prediction are used to achieve more accurate tracking.

1. Introduction

Quantum control has become an important topic in quantum information [1, 2], molecular chemistry [3], and atomic physics [4]. Many control methods, including optimal control [5], Lyapunov control [6], learning control [7], feedback control [8], and incoherent control [9, 10], have been used in controller design of quantum systems. Our recent work [11, 12] has extended the classical probability density function (PDF) control method into quantum area. Based on classical PDF control, there is also a developing research area on Shannon entropy control, which has achieved good performance in classical systems, such as stochastic control [13, 14], networked control [15], and biological control [16]. The extension of Shannon entropy control into quantum area may also enhance quantum control performance.

Shannon entropy in atomic calculations has further been related to various properties such as atomic ionization potential [17], molecular geometric parameters [18], chemical similarity of different functional groups [19], characteristics of correlation methods for global delocalizations [20], molecular reaction paths [21], orbital-based kinetic theory [22], highly excited states of single-particle systems [23], and nature of chemical bonds [24]. The consistency of the Shannon entropy when applied to outcomes of quantum experiments has been analyzed [25], and it is shown that Shannon entropy is fully consistent and its properties are never violated in quantum settings.

In the recent research about quantum sliding-mode control (SMC) [26, 27], a sliding mode is defined based on the fidelity with a desired eigenstate, and the goal is to maintain the state in the mode or drive it back into the mode after measurement. In fact, the fidelity here is directly related to Shannon entropy. There is also research about coherent control based on tracking control for two-level systems [28]. Since coherence corresponds to large entropy, while fidelity corresponds to small entropy, we can directly control the entropy to achieve the goal. If the entropy can track a desired trajectory, the state will be able to slide among different modes, rather than in one mode in the existing quantum SMC. For n-level systems which cannot be depicted by Bloch sphere, such method can also provide a systematic way to maintain fidelity or coherence.

For the biological and physiological datasets, quantifying disorder of the system has become popular as an intense area of promising recent research. In the recent study of a complexity measure for nonstationary signals [16], Shannon entropy has been used to distinguish “healthy” from “unhealthy” biological signals. The study has quantified the information evolution of transitions associated with probabilities assigned to each state, with a goal of providing single value (an entropy) to describe the information content. Similar approach can be adopted to systems where the change in parameter would be indicative of a change in the "health" of the system. For example, in the recent research about information theoretic measures of the electron correlation for
both continuous [29] and discrete [30] cases, it is shown that
Shannon entropy can also provide a new way to calculate
electron correlation energy more accurately. An accurate
description of atomic and molecular properties requires an
explicit account of electron correlation, while there is no ope-
rator in quantum mechanics whose measurement gives the
correlation energy. Since strong correlation corresponds
to large entropy, we can also use Shannon entropy as a new
approach to control quantum correlation.

Quantum von Neumann entropy is a good measure of
entanglement, and it will reduce to Shannon entropy for the
pure state case. It can provide a real-time noise observation
and a systematic guideline to make reasonable choice of
control strategy. The von Neumann entropy is just a measure
of the purity of the given density matrix without explicit ref-
ere to information contained in individual measurements
[31]. While quantum Shannon entropy can reveal a great deal
of information from the perspective of geometrical changes to
the density [21], it shows interesting features about the bond
forming and breaking process that are not apparent from
the conventional reaction energy profile. Recent research has
studied how to image and manipulate the shape of electronic
wavefunction [32] and how to directly measure the quantum
wavefunction for photons [33]. If the probability density
function can be well measured and controlled in the future,
we can directly control the detailed spatial distribution for
both pure and mixed states. Sometimes, the detailed distribu-
tion may not be important, while we only need to make the
distribution more ordered or disordered. This also calls for
the control of the uncertainty, which can be directly reflected
by Shannon entropy.

This paper provides two primary methods to steer the dis-
crete and continuous quantum Shannon entropy via quantum
PDF control. And for the discrete case, a method based on
discretization approximation is provided which can directly
control the entropy and achieve more accurate performance.
This paper is organized as follows. Section 2 presents the basic
quantum control model and the definitions of both discrete
and continuous quantum Shannon entropy. Sections 3 and 4
provide the controller design methods based on PDF control
for discrete and continuous entropy, respectively. Section 5
provides a direct control method for discrete entropy based
on discretization approximation. Section 6 shows the num-
erical simulation examples. Concluding remarks are given in
Section 7.

2. Preliminary

In quantum control, the state of a closed quantum system
is represented by a state vector (wavefunction) \( \psi(x, t) \) in a
Hilbert space. Here, for the space variable we only consider
one-dimensional position variable \( x \). The evolution of the
state obeys the Schrödinger equation:

\[
\frac{\partial \psi(x, t)}{\partial t} = \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + U(x, t) \right) \psi(x, t),
\]

where \( i = \sqrt{-1} \) and the external potential field \( U(x, t) \in \mathbb{R} \) is
taken as the control term. For an infinite dimensional quan-
tum system, the wavefunction \( \psi(x, t) \) is the superposition
of free Hamiltonian's eigenstates \( \psi_i(x) \):

\[
\psi(x, t) = \sum_{i=1}^{\infty} c_i(t) \psi_i(x),
\]

where both the wavefunction and the coefficients should be
normalized:

\[
\int_{-\infty}^{\infty} |\psi(x, t)|^2 dx = \sum_{i=1}^{\infty} |c_i(t)|^2 = 1.
\]

Defining the state of the system as follows:

\[
C(t) = [c_1(t), c_2(t), \ldots, c_n(t), \ldots]^T,
\]

and the Schrödinger equation can be written as follows:

\[
\dot{C}(t) = \begin{bmatrix} A + \sum_{i=1}^{k} B_i U_i(t) \end{bmatrix} C(t),
\]

where both \( A \) and \( B_i \) are skew-Hermitian matrices. If the case
with only one control \( U(1) \) can be well solved, it will be easier
for multiple control cases. So, this paper only considers the
following case with one control:

\[
\dot{C}(t) = AC(t) + BU(t)C(t).
\]

Assuming a system that consists of \( n \) states, in which the
probability for the \( i \)th state to happen is \( p_i \), the traditional
discrete Shannon entropy in information science is defined as
follows:

\[
S_d = -\sum_{i=1}^{n} p_i \ln p_i,
\]

which shows the degree of randomness of the system. For
example, when \( p_1 = p_2 = \cdots = p_n = 1/n \), every state happens
in the equal probability, which is a random system. In this
situation, the Shannon entropy takes its maximum value \( \ln n \).
If \( p_i = 1 \), the system is completely predictable; that is, the
first state always happens, and the entropy takes its minimum
value 0. We can also regard the entropy as the superposition
of the uncertainties \( \ln(1/p_i) \) because larger probability can
lead to smaller uncertainty. Similarly, the discrete quantum
Shannon entropy can be defined as follows:

\[
S_d(t) = -\sum_{i=1}^{\infty} |c_i(t)|^2 \ln |c_i(t)|^2,
\]

where \( |c_i(t)|^2 \) is the probability that the superposition state
collapses to the \( i \)th eigenstate upon quantum measurement.
Next, for the continuous case, Shannon proposed that the
entropy for a system with a probability distribution \( p(x) \) in
one dimension could be characterized by the following:

\[
S_c = -\int p(x) \ln p(x) \, dx, \quad \int p(x) \, dx = 1.
\]
which measures the delocalization or the lack of structure in the respective distribution. Thus, the entropy is maximal for uniform distribution and is minimal when the uncertainty about the structure of the distribution is minimal. Since the quantum probability density can be denoted by a continuous function \( |\psi(x, t)|^2 \), we can define continuous quantum Shannon entropy as follows:

\[
S_c(t) = -\int_{-\infty}^{\infty} |\psi(x, t)|^2 \ln |\psi(x, t)|^2 \, dx,
\]

(10)

where integral can be used to deal with continuous probability distribution. Our goal is to drive the entropy from any initial value to any target.

### 3. Controller Design for Discrete Entropy Based on PDF Control

Here, we consider finite dimensional quantum systems. From definition (8), we know that the discrete entropy satisfies the following:

\[
S_d(t) = -\sum_{i=1}^{n} |c_i(t)|^2 \ln |c_i(t)|^2 \geq 0.
\]

(11)

It is clear that when \( |c_i(t)|^2 = |c_i(t)|^2 = \cdots = |c_n(t)|^2 = 1/n \), \( S_d(t) \) reaches its maximum \( \ln n \). \( S_d(t) \) reaches its minimum 0 when

\[
|c_i(t)|^2 = \begin{cases} 
1, & i = k, \\
0, & i \neq k,
\end{cases}
\]

(12)

where \( k \) is a given integer. This conclusion can be proved using the following fact:

\[
\lim_{x \to 0} x \ln x = \lim_{x \to 0} \frac{\ln x}{1/x} = \lim_{x \to 0} \frac{(d/dx)(\ln x)}{(1/x)} = \lim_{x \to 0} (-x) = 0.
\]

(13)

The control of \( S_d(t) \) can be realized by controlling the probability density \( |c_i(t)|^2 \).

Denote the target of \( C(t) \) as follows:

\[
C = [c_1, c_2, \ldots, c_n]^T,
\]

(14)

which satisfies the normalization condition

\[
\sum_{i=1}^{n} |c_i|^2 = 1.
\]

(15)

There are several methods [6, 34] to reach the target under some assumptions, though the asymptotic stability may not be guaranteed. Here, we provide another method which can deal with any final condition without guaranteeing the asymptotic stability. First, we define the error as follows:

\[
e(t) = \sum_{i=1}^{n} |c_i(t) - c_i|^2.
\]

(16)

In order to make the error decrease, we let

\[
\dot{e}(t) = -ke(t),
\]

(17)

where \( k \in \mathbb{R}^+ \) can be preselected. Substituting (3), (14), and (15) into (16) we have the following:

\[
e(t) = \sum_{i=1}^{n} |c_i(t) - c_i| \geq 0.
\]

\[
ge(t) = \sum_{i=1}^{n} |c_i(t)|^2 + \sum_{i=1}^{n} |c_i|^2 - \sum_{i=1}^{n} [c_i^* c_i(t) + c_i^* c_i(t) c_i]
\]

\[
= 2 - 2\sum_{i=1}^{n} \Re [c_i^* c_i(t)] = 2 - 2\Re \left[ \sum_{i=1}^{n} c_i^* c_i(t) \right]
\]

(18)

where \( C^+ = (C^*)^T \). Then we can obtain the following relationship based on (6), (17), and (18):

\[
\dot{e}(t) = -2\Re \left[ C^+ \dot{C}(t) \right]
\]

\[
= -2\Re \left[ C^* [A + U(t)B] C(t) \right]
\]

\[
= -2\Re \left[ C^* A C(t) \right] - 2U(t) \Re \left[ C^* B C(t) \right]
\]

\[
= -k \left[ 2 - 2\Re \left[ C^* C(t) \right] \right].
\]

(19)

From (19), we can get the following controller:

\[
U(t) = \frac{k - \Re \left[ C^* [A + kI] C(t) \right]}{\Re \left[ C^* B C(t) \right]}.
\]

(20)

This is the desired controller which can make the error decrease.

When the state has reached its target, in order to keep it unchanged, we can do the following calculation about the derivative of the probability density:
where "\(\circ\)" is defined as follows, which means the corresponding elements are multiplied:

\[
\begin{bmatrix}
    a_1 \\
    a_2 \\
    \vdots \\
    a_n
\end{bmatrix} \circ \begin{bmatrix}
    b_1 \\
    b_2 \\
    \vdots \\
    b_n
\end{bmatrix} = \begin{bmatrix}
    a_1b_1 \\
    a_2b_2 \\
    \vdots \\
    a_nb_n
\end{bmatrix}.
\] (22)

From (21), it is easy to find that in order to keep the probability constant, we only need the following:

\[
\Re \left[ AC(t) \circ C^*(t) \right] + U(t) \Re \left[ BC(t) \circ C^*(t) \right] = \begin{bmatrix}
    0 \\
    0 \\
    \vdots \\
    0
\end{bmatrix} + \begin{bmatrix}
    0 \\
    0 \\
    \vdots \\
    0
\end{bmatrix}_{m \times 1}.
\] (23)

When \(A\) is diagonal, all the elements in \(A\) should be pure imaginary because \(A\) is skew-Hermitian. Assuming \(A = \text{diag}[a_{11}, a_{22}, \ldots, a_{nn}]\) \((a_{ij} \in \mathbb{R})\), we have the following:

\[
\Re \left[ AC(t) \circ C^*(t) \right] = \Re \left\{ [a_{11}|c_1(t)|^2 + a_{22}|c_2(t)|^2 + \ldots + a_{nn}|c_n(t)|^2] \right\} = 0.
\] (24)

Hence, once the system's entropy reaches the target, we can use \(U(t) = 0\) to maintain the entropy unchanged. For other quantum systems with nondiagonal \(A\), it is not easy to keep the entropy unchanged with (23). Then we will develop an approximation method in Section 5 to achieve good performance.

4. Controller Design for Continuous Entropy Based on PDF Control

From definition (10), we know \(S_q(t) \geq 0\). It is easy to prove that \(S_q(t)\) can reach its maximum when the probability distribution \(|\psi(x,t)|^2\) is a uniform distribution and can reach its minimum when the uncertainty about the structure of the distribution is minimal, for example, a delta-like distribution. We can control the continuous entropy by controlling \(|\psi(x,t)|^2\).

Define the target distribution of \(\psi(x,t)\) as \(\psi_d(x)\) which satisfies the following:

\[
\int_{-\infty}^{\infty} |\psi_d(x)|^2 dx = 1.
\] (25)

The error can be defined as follows:

\[
e(t) = \int_{-\infty}^{\infty} |\psi(x,t) - \psi_d(x)|^2 dx.
\] (26)

The goal is to make the error decrease in this way:

\[
\dot{e}(t) = -ke(t). \quad (27)
\]

Based on (3) and (25), we can rewrite \(e(t)\) as follows:

\[
e(t) = \int_{-\infty}^{\infty} \left[ \psi^*(x,t) - \psi^d(x) \right] \left[ \psi(x,t) - \psi_d(x) \right] dx
\]

\[
= \int_{-\infty}^{\infty} |\psi(x,t)|^2 dx + \int_{-\infty}^{\infty} |\psi_d(x)|^2 dx
\]

\[
- \int_{-\infty}^{\infty} \left[ \psi^*(x,t) \psi_d(x) + \psi^d(x) \psi(x,t) \right] dx
\]

\[
= 2 - 2 \int_{-\infty}^{\infty} \Re \left[ \psi^d(x) \psi(x,t) \right] dx.
\] (28)

Then we can obtain the following relationship based on (1), (27), and (28):

\[
\dot{e}(t) = -2 \int_{-\infty}^{\infty} \Re \left[ \psi^d(x) \psi(x,t) \right] dx
\]

\[
= -2 \int_{-\infty}^{\infty} \Re \left[ \psi^d(x) \psi(x,t) \right] dx
\]

\[
= -2 \int_{-\infty}^{\infty} \Re \left[ \psi^d(x) \psi(x,t) \right] dx
\]

\[
= -2 \int_{-\infty}^{\infty} \left[ \psi^d(x) \psi(x,t) \right] dx
\]

\[
= -k \left\{ 2 - 2 \int_{-\infty}^{\infty} \Re \left[ \psi^d(x) \psi(x,t) \right] dx \right\}.
\] (29)

From (29), we can get the following controller:

\[
U(t) = \left( \frac{\hbar^2}{2m} \int_{-\infty}^{\infty} \Im \left[ \psi^d(x) \frac{\partial^2 \psi(x,t)}{\partial x^2} \right] dx \right.
\]

\[
- k h \int_{-\infty}^{\infty} \Re \left[ \psi^d(x) \psi(x,t) \right] dx + k \hbar
\]

\[
\times \left( \int_{-\infty}^{\infty} \Im \left[ \psi^d(x) \psi(x,t) \right] dx \right)^{-1}.
\] (30)

This is the desired controller which can make the error decrease when applied to the quantum system. We can substitute (30) into the Schrödinger equation (1) to solve \(U(t)\) out because only \(\psi(x,t)\) and \(U(t)\) are unknown. This task can be numerically accomplished by computer simulation or discretization. Moreover, in practice, some methods have been developed for the real-time measurement of quantum PDF.
under some special cases [32, 35]. If the quantum PDF can be measured online in the future, we can directly measure \( \psi(x,t) \) and calculate \( U(t) \) with (30). When \( \psi(x,t) \rightarrow \psi_d(x) \), \( U(t) \) will not be asymptotic stable. We can design an external field to make \( \psi(x,t) \) unchanged when it is near to \( \psi_d(x) \) at time \( t_f \). To make \( \psi(x,t) \) unchanged is just to make

\[
\forall t > t_f, \quad \psi(x,t) = \psi(x,t_f).
\]

Substituting (31) into the Schrödinger equation (1) we obtain the following:

\[
0 = -\frac{\hbar^2}{2m} \frac{d^2 \psi(x,t_f)}{dx^2} + U(x,t) \psi(x,t_f),
\]

which gives the following:

\[
U(x,t) = U(x) = \frac{\hbar^2}{2m \psi(x,t_f)} \frac{d^2 \psi(x,t_f)}{dx^2}.
\]

Such a field will keep \( \psi(x,t) \) constant.

5. Controller Design for Discrete Entropy Based on Discretization Approximation

In the above two methods, the entropy does not truly enter the control procedure and cannot be driven to the target at any prespecified time. To achieve more direct and accurate control, we can adopt discretization to clarify the relationship between the entropy and the controller.

Assuming the sampling period is \( T \), the control model (6) with dimension \( n \) can be descretized as follows:

\[
\frac{C(T) - C(0)}{T} = AC(0) + BU(0)C(0),
\]

where \( C(0) \) is the initial state, \( C(T) \) is the state at time \( T \), and \( U(0) \) is the external potential field which will remain constant in the first sampling period \( T \). Then we have the following:

\[
C(T) = (I + TA)C(0) + TBU(0)C(0),
\]

where \( I \) is the identity matrix with dimension \( n \). For finite dimensional quantum systems, the derivative of the discrete entropy (8) is as follows:

\[
\frac{dS_d(t)}{dt} = - \sum_{i=1}^{n} \left[ \ln |c_i(t)|^2 + 1 \right] \frac{d|c_i(t)|^2}{dt}
\]

\[
= - \sum_{i=1}^{n} \frac{d|c_i(t)|^2}{dt} \ln |c_i(t)|^2 - \sum_{i=1}^{n} \frac{d|c_i(t)|^2}{dt}.
\]

Hence (36) can be changed into the following:

\[
\frac{dS_d(t)}{dt} = - \sum_{i=1}^{n} \frac{d|c_i(t)|^2}{dt} \ln |c_i(t)|^2.
\]

We discretize (38) as

\[
\frac{S_d(T) - S_d(0)}{T} = - \sum_{i=1}^{n} \frac{|c_i(t)|^2 - |c_i(0)|^2}{T} \ln |c_i(0)|^2,
\]

which implies

\[
S_d(T) - S_d(0)
\]

\[
= - \sum_{i=1}^{n} |c_i(t)|^2 \ln |c_i(0)|^2 + \sum_{i=1}^{n} |c_i(0)|^2 \ln |c_i(0)|^2.
\]

It is clear that

\[
S_d(0) = - \sum_{i=1}^{n} |c_i(0)|^2 \ln |c_i(0)|^2.
\]

Substituting (41) into (40) leads to the following:

\[
S_d(T) = - \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(0)|^2.
\]

Here, we use \( - \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(0)|^2 \) to approximate \( - \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(T)|^2 \). The following theorem shows that not only the approximation is feasible, but also the approximation error is an infinitesimal of higher order than the change of probability under small change of the probability.

**Theorem 1.** When \( |c_i(0)|^2 \neq 0 \) (for all \( i \)) holds, if the probability change is very small (for all \( i \), \( |c_i(T)|^2 - |c_i(0)|^2 \rightarrow 0 \)), \( S_d(T) = - \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(T)|^2 (T \rightarrow 0) \) can be approximated by \( - \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(0)|^2 \), and the approximation error \( e = \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(T)|^2 - \sum_{i=1}^{n} |c_i(T)|^2 \ln |c_i(0)|^2 \) is an infinitesimal of higher order than the probability change \( \sum_{i=1}^{n} |c_i(T)|^2 - |c_i(0)|^2 \).

**Proof.** Assume \( |c_i(0)|^2 = p_i \neq 0 \), \( |c_i(T)|^2 - |c_i(0)|^2 = \Delta_i \), and \( e \) can be written as follows:

\[
eq \sum_{i=1}^{n} (p_i + \Delta_i) \ln (p_i + \Delta_i) - \sum_{i=1}^{n} (p_i + \Delta_i) \ln p_i
\]

\[
= \sum_{i=1}^{n} (p_i + \Delta_i) \ln \frac{p_i + \Delta_i}{p_i}.
\]
It is clear that
\[
\lim_{\Delta_i \to 0} \frac{(p_i + \Delta_i) \ln \left( \frac{(p_i + \Delta_i)}{p_i} \right)}{\Delta_i} = \lim_{\Delta_i \to 0} \frac{\ln \left( \frac{(p_i + \Delta_i)}{p_i} \right)}{\Delta_i / (p_i + \Delta_i)} = \lim_{\Delta_i \to 0} \left( \frac{d}{d\Delta_i} \ln \left( \frac{(p_i + \Delta_i)}{p_i} \right) \right) (\Delta_i / (p_i + \Delta_i))
\]
which implies
\[
\lim_{\Delta_i \to 0} \frac{(p_i / (p_i + \Delta_i)) \cdot (1/p_i)}{(p_i + \Delta_i - \Delta_i) / (p_i + \Delta_i)^2} = \lim_{\Delta_i \to 0} \left( 1 + \Delta_i / p_i \right) = 1,
\]
so we can get \( \lim_{\Delta_i \to 0} (p_i + \Delta_i) \ln \left( \frac{(p_i + \Delta_i)}{p_i} \right) = \lim_{\Delta_i \to 0} \Delta_i \), which implies \( \lim_{\Delta_i \to 0} e = \lim_{\Delta_i \to 0} \sum_{i=1}^{n} \Delta_i = 0 \). Since the limit of the approximation error is zero, we can say the approximation is feasible. Moreover, we have the following:
\[
\lim_{\Delta_i \to 0} \sum_{i=1}^{n} \| c_i (T) \|^2 - | c_i (0) |^2 = 0.
\]
Hence,
\[
e = o \left( \sum_{i=1}^{n} \| c_i (T) \|^2 - | c_i (0) |^2 \right).
\]

Theorem 1 allows us to use (42) to approximate the entropy after change. Here, for simplicity we define a row vector:
\[
D = \left[ -\ln | c_1 (0) |^2, -\ln | c_2 (0) |^2, \ldots, -\ln | c_n (0) |^2 \right] = [d_1, d_2, \ldots, d_n] \in \mathbb{R}^{1 \times n}.
\]
Since \( 0 \leq | c_i (0) |^2 \leq 1 \), we know \( d_i \geq 0 \). Substituting (47) into (42) leads to the following:
\[
S_d (T) = D \left[ C(T) \circ C^* (T) \right] = D \left[ (I + TA) C(0) + U(0) TBC (0) \right] \circ [(I + TA^*) C^* (0) + U(0) TB C^* (0)]
\]
\[
= D \left[ (I + TA) C(0) \right] \circ \left[ (I + TA^*) C^* (0) \right] + U^2 (0) TBC (0) \circ TB C^* (0)
\]
\[
+ U (0) \left[ TBC (0) \circ (I + TA^*) C^* (0) \right] + U (0) \left[ TBC (0) \circ (I + TA) C (0) \circ TB C^* (0) \right].
\]
Define
\[
M = TBC (0) \circ TB C^* (0) \in \mathbb{R}^{1 \times 1},
\]
\[
N = TBC (0) \circ (I + TA^*) C^* (0) \in \mathbb{R}^{1 \times 1},
\]
\[
K = (I + TA) C (0) \circ (I + TA^*) C^* (0) \in \mathbb{R}^{1 \times 1},
\]
which can change (48) into the following:
\[
S_d (T) = U^2 (0) DM + U(0) DN + DK.
\]
It is clear that all the elements in \( M \) and \( K \) are nonnegative, which lead to \( DM \geq 0 \) and \( DK \geq 0 \). When \( DM = 0 \), to make the entropy in (50) reach its target, we can simply choose \( U(0) = (S_d (T) - DK) / DN \). But in most cases we have \( DM > 0 \), and from (50) the one-step controller can be calculated as follows:
\[
U (0) = \frac{-DN \pm \sqrt{(DN)^2 - 4DM [DK - S_d (T)]}}{2DM}.
\]
Here, the selection of plus and minus depends on the value of \( |U(0)| \), and detailed discussions can be found in Section 6.1. Since \( U(0) \) belongs to the real domain, we have \( (DN)^2 - 4DM [DK - S_d (T)] \geq 0 \), which leads to the following:
\[
S_d (T) \geq DK - \frac{(DN)^2}{4DM}.
\]
This means that \( S_d (T) \) has a lower bound. Proposition 2 shows that the lower bound is nonnegative.

Proof. Define two column-vectors as follows:
\[
x \triangleq TBC (0) = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \in \mathbb{C}^{n \times 1},
\]
\[
y \triangleq (I + TA) C (0) = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \in \mathbb{C}^{n \times 1},
\]
and \( M, N, \) and \( K \) can be rewritten as follows:
\[
M = x \circ x^* = \begin{bmatrix} |x_1|^2 \\ |x_2|^2 \\ \vdots \\ |x_n|^2 \end{bmatrix},
\]
\[
N = x \circ y^* + y \circ x^* = 2 \Re \{ x \circ y^* \} = \begin{bmatrix} \Re (x_1 y_1^*) \\ \Re (x_2 y_2^*) \\ \vdots \\ \Re (x_n y_n^*) \end{bmatrix},
\]
\[
K = y \circ y^* = \begin{bmatrix} |y_1|^2 \\ |y_2|^2 \\ \vdots \\ |y_n|^2 \end{bmatrix}.
\]
We can do the following calculation:

\[
(DM)(DK) - \frac{(DN)^2}{4}
\]

\[
= \left(\sum_{i=1}^{n}d_i |x_i|^2\right) \left(\sum_{i=1}^{n}d_j |y_j|^2\right) - \left[\sum_{i=1}^{n} d_i \mathcal{R}(x_i y_i^*)\right]^2
\]

\[
= \sum_{i=1}^{n} \sum_{j=1}^{n} d_i d_j |x_i y_j^*|^2 - \mathcal{R}(x_i y_j^*) \mathcal{R}(x_j y_i^*)
\]

\[
\geq 0.
\]

(56)

For \(i = j\),

\[
d_i d_j \left[|x_i y_i^*|^2 - \mathcal{R}(x_i y_i^*) \mathcal{R}(x_j y_j^*)\right]
\]

\[
= d_i^2 \left[|x_i y_i^*|^2 - |\mathcal{R}(x_i y_i^*)|^2\right] \geq 0.
\]

(57)

For \(i \neq j\),

\[
d_i d_j \left[|x_i y_j^*|^2 - \mathcal{R}(x_i y_j^*) \mathcal{R}(x_j y_i^*)\right]
\]

\[
+ d_i d_j \left[|x_i y_i^*|^2 - \mathcal{R}(x_j y_i^*) \mathcal{R}(x_j y_j^*)\right]
\]

\[
= d_i d_j \left[|x_i y_i^*|^2 + |x_j y_j^*|^2 - 2 \mathcal{R}(x_i y_j^*) \mathcal{R}(x_j y_j^*)\right]
\]

\[
= d_i d_j \left[|x_i y_i^*|^2 - 2|y_i|^2 |x_j|^2 + |x_j|^2 |x_i|^2\right]
\]

\[
+ 2 |x_i y_i^*|^2 |x_j|^2 - 2 \mathcal{R}(x_i y_j^*) |x_j y_j^*| |x_i y_i^*|
\]

\[
+ 2 |\mathcal{R}(x_i y_j^*)| |\mathcal{R}(x_j y_j^*)| - 2 \mathcal{R}(x_i y_j^*) \mathcal{R}(x_j y_j^*)
\]

\[
\geq 0.
\]

(58)

So, \((DM)(DK) - ((DN)^2/4) \geq 0\), which implies \(DK - ((DN)^2/4DM) \geq 0\). \(\Box\)

Proposition 2 shows that \(S_d(T)\) has a nonnegative lower bound, which will affect the selection of the target. When the lower bound is smaller than \(S_d(0)\), the entropy can be reduced; otherwise, the entropy cannot be reduced in time \(T\). However, it is possible to reduce the entropy after \(T\) using suitable control, which will be demonstrated by simulation in Section 6.1. This conclusion coincides with our common sense. Just as we know, it is always easy to make a system disordered, but it is not always easy to make a system ordered. To investigate when the entropy cannot be reduced, we can calculate the gap between the lower bound and \(S_d(0)\) as follows:

\[
S_d(0) - \left[ DK - \frac{(DN)^2}{4DM} \right]
\]

\[
= \frac{1}{DM} \left[ \frac{(DN)^2}{4} - DM \left[ DK - S_d(0) \right] \right]
\]

\[
= \frac{1}{D [TBC(0) * TB^* C^* (0)]}
\]

\[
\times \left\{ \left[ \frac{1}{4} \mathcal{R} \left[ TBC(0) * (I + TA^*) C^* (0) \right] \right]^2
\]

\[
- D \left[ TBC(0) * TB^* C^* (0) \right]
\]

\[
\times \left[ D \left[ (I + TA) C(0) * (I + TA^*) C^* (0) \right]
\]

\[
- D \left[ C(0) * C^* (0) \right] \right\}
\]

\[
= \frac{1}{T^2 D [BC(0) * B^* C^* (0)]}
\]

\[
\times \left\{ \left[ D \mathcal{R} \left[ TBC(0) * (I + TA^*) C^* (0) \right] \right]^2
\]

\[
- D \left[ TBC(0) * TB^* C^* (0) \right]
\]

\[
\times D \left[ TAC(0) * C^* (0) + TC(0) * A^* C^* (0) \right]
\]

\[
+ T^2 AC(0) * A^* C^* (0) \right\}
\]

\[
= \frac{T^2}{D [BC(0) * B^* C^* (0)]}
\]

\[
\times \left\{ \left[ D \mathcal{R} \left[ BC(0) * (I + TA^*) C^* (0) \right] \right]^2
\]

\[
- D \left[ BC(0) * B^* C^* (0) \right]
\]

\[
\times D \left[ 2T \mathcal{R} \left[ AC(0) * C^* (0) \right]
\]

\[
+ T^2 AC(0) * A^* C^* (0) \right\}
\]

\[
= \frac{1}{D [BC(0) * B^* C^* (0)]}
\]

\[
\times \left\{ \left[ D \mathcal{R} \left[ BC(0) * C^* (0) \right] \right]^2
\]

\[
+ T D \mathcal{R} \left[ BC(0) * A^* C^* (0) \right] \right\}
\]

\[
- 2TD \left[ BC(0) * B^* C^* (0) \right] D \mathcal{R} \left[ AC(0) * C^* (0) \right]
\]

\[
- T^2 D \left[ BC(0) * B^* C^* (0) \right] D \left[ AC(0) * A^* C^* (0) \right] \right\}.
\]

(59)

Let

\[
S_d(0) - \left[ DK - \frac{(DN)^2}{4DM} \right] = \frac{aT^2 + bT + c}{D [BC(0) * B^* C^* (0)]}.
\]

(60)
\[ a = \{D \mathfrak{R} [BC(0) \circ AC^*(0)]\}^2 \]

\[ b = 2D \mathfrak{R} [BC(0) \circ C^*(0)] D \mathfrak{R} [BC(0) \circ AC^*(0)], \]

\[ c = \{D \mathfrak{R} [BC(0) \circ C^*(0)]\}^2. \]

From \(D[BC(0) \circ B^*C^*(0)] \geq 0\), we know that the entropy cannot be reduced when \(\lim_{T \to 0} (aT^2 + bT + c) \leq 0\). The following proposition shows that \(a \leq 0\).
For $i \neq j$,
\[
\begin{align*}
d_{i,j} &\left[ R(p_i q_j^*) R(p_j q_i^*) - |p_i|^2 |q_j|^2 \right] \\
&\quad + d_{j,i} \left[ R(p_j q_i^*) R(p_i q_j^*) - |p_j|^2 |q_i|^2 \right] \\
&= d_{i,j} \left[ 2 R(p_i q_j^*) R(p_j q_i^*) - |p_i|^2 |q_j|^2 - |p_j|^2 |q_i|^2 \right] \\
&\leq d_{i,j} \left[ 2 |R(p_i q_j^*)| |R(p_j q_i^*)| - |p_i|^2 |q_j|^2 - |p_j|^2 |q_i|^2 \right] \\
&\leq d_{i,j} \left[ 2 |p_i q_j^*||p_j q_i^*| - |p_i|^2 |q_j|^2 - |p_j|^2 |q_i|^2 \right] \\
&= -d_{i,j} \left( |p_i q_j^*| - |p_j q_i^*|^2 \right)^2 \leq 0.
\end{align*}
\]

We can conclude that $a \leq 0$. \hfill \Box

Based on Proposition 3, we can find out under what conditions the entropy cannot be reduced, which is shown in Theorem 4.

\textbf{Theorem 4.} The entropy cannot be reduced in very small time $T$ when
\[\sum (AC) < 0, \quad D\Re [(BC) \circ (C^*)] = 0. \tag{67}\]

\textbf{Proof.} From (61) we know $c \geq 0$. When $c > 0$, it is clear that $\lim_{T \to 0} (aT^2 + bT + c) > 0$, which means that the entropy can be reduced. When $c = 0$ and $a = 0$, $\lim_{T \to 0} (aT^2 + bT + c) \leq 0$ is true only when $b \leq 0$. When $c = 0$ and $a < 0$, from Figure 1, we can see that $\lim_{T \to 0} (aT^2 + bT + c) \leq 0$ only holds when $b \leq 0$.

So the conditions under which the entropy can only be reduced are $c = 0$ and $b \leq 0$. From (61) we know $c = 0$ implies $D\Re [BC(0) \circ C^*(0)] = 0$ which yields $b = -2D[BC(0) \circ B^C C^*(0)] D\Re [(AC(0) \circ C^*)]$. From $D\Re [BC(0) \circ B^C C^*(0)] \geq 0$, we know that, to get $b \leq 0$, we only need $D\Re [AC(0) \circ C^*(0)] \geq 0$. We can conclude the result in Theorem 4. \hfill \Box

Theorem 4 gives the conditions under which the entropy cannot be reduced. During practical control process, we do not need to do the calculations in (67) at every step. This is because if one wants to reduce the entropy when it cannot be reduced, the selection of $S_d(T)$ must be smaller than its lower bound, which makes $(DN)^2 - 4DM[D-K - S_d(T)] < 0$, and the controller (51) will be unsolvable. Another question is that, even when the entropy can be reduced, we cannot reduce it below the lower bound in one time step $T$. In order to reduce it below the lower bound, multistep tracking can be adopted since Theorem 1 only holds for small change of the probability. Although fast probability change may lead to fast entropy decreasing, it cannot be tracked and approximated with Theorem 1.

We can show the essence of the algorithm in Figure 2 based on two-level quantum systems. Assuming $|c_i(t)|^2 = p$,
the entropy of two-level systems becomes $S = -p \ln p - (1-p) \ln(1-p)$. The relationship between entropy and probability can be depicted in Figure 2.

For arbitrary point $A$, when the system goes from $A$ to $A'$, the probability change can be denoted as $\Delta p = p_{A'} - p_A$. If we denote the entropy at $A'$ as $S_{A'}$ and approximate it with $S_{A''}$, the approximation error $e = S_{A'} - S_{A''}$ should satisfy $\lim_{\Delta p \to 0} (e/\Delta p) = 0$. Obviously there will be some delay in such an approximation. Hence, in Section 6.2, we will use prediction to achieve more accurate tracking.

It should be noted that for the entropy's maximum point $B$ and minimum points $C$ and $D$, our algorithm cannot be applied. For point $B$, we have $dS/dp = 0$ and $S_{B''} = S_{B'}$, so the entropy will not change under the approximation of $S_{B''}$. For quantum systems with $n$ levels, the maximum point satisfies $|c_i(0)|^2 = (1/n)$ (for all $i$), so we can get $S_d(T) = -\sum_{i=1}^n |c_i(T)|^2 \ln |c_i(0)|^2 = -\sum_{i=1}^n |c_i(T)|^2 \ln(1/n) = \ln n \cdot \sum_{i=1}^n |c_i(T)|^2 = \ln n = S_d(0)$, which will not change the entropy either. For point $C$ we have $dS/dp = +\infty$, $\lim_{\Delta p \to 0} (e/\Delta p) = -\infty$, and for point $D$ we have $dS/dp = -\infty$, $\lim_{\Delta p \to 0} (e/\Delta p) = +\infty$, which make the algorithm unfeasible. For three-level systems, when the entropy is at its minimum, one of $|c_i(t)|^2$ ($i = 1, 2, 3$) must be 1, and the others must be 0. Assume the vector $[|c_1(t)|^2, |c_2(t)|^2, |c_3(t)|^2]$ goes from $[1, 0, 0]$ to $[1 - \Delta_1 - \Delta_2, \Delta_1, \Delta_2]$ ($\Delta_1 > 0, \Delta_2 > 0$). Such a process is equivalent to $[1, 0, 0] \to [1 - \Delta_1 - \Delta_2, \Delta_1 + \Delta_2, 0] \to [1 - \Delta_1, \Delta_2, \Delta_2]$. If we denote the errors in each
It is easy to verify that
\[
\lim_{\Delta_1 + \Delta_2 \to 0} \frac{e_1 + e_2}{2(\Delta_1 + \Delta_2)} = \frac{e_1}{2(\Delta_1 + \Delta_2)} + \frac{e_2}{2(\Delta_1 + \Delta_2)},
\]
\[
\lim_{\Delta_1 + \Delta_2 \to 0} \frac{\Delta_2}{\Delta_1 + \Delta_2} = \frac{e_2}{\Delta_1 + \Delta_2} - \lim_{\Delta_1 + \Delta_2 \to 0} \frac{\Delta_2}{2(\Delta_1 + \Delta_2)} = -\infty + \frac{\Delta_2}{\Delta_1 + \Delta_2} (-\infty) = -\infty.
\]

The same conclusion holds for quantum systems with more than three levels.

6. Simulation Examples

In order to illustrate the effectiveness of our algorithm, we present simulation examples on both two-level and three-level quantum systems.

6.1. Simulation on a Two-Level System. Consider the system
\[
\begin{bmatrix}
c_1(t) \\
c_2(t)
\end{bmatrix} = \begin{bmatrix} -i & 0 \\ 0 & i \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} U(t) \begin{bmatrix} c_1(t) \\
c_2(t)
\end{bmatrix}. \tag{69}
\]

It is easy to verify that $DM = -T^2[|c_1(0)|^2 \ln |c_2(0)|^2 + |c_2(0)|^2 \ln |c_1(0)|^2] > 0$, so we should always use (51) to calculate $U(0)$. It is easy to obtain the following:
\[
D\Re [AC(0) + C^*(0)] = 0,
\]
\[
D\Re [BC(0) + C^*(0)] = \Re [c_1(0) c_2^*(0) \ln \frac{|c_2(0)|^2}{|c_1(0)|^2}]. \tag{70}
\]

If the entropy is not at its maximum or minimum, we have $\ln(|c_2(0)|^2/|c_1(0)|^2) \neq 0$ or $\pm \infty$, and, from Theorem 4, we know that the condition under which the entropy cannot be reduced is as follows:
\[
\Re [c_1(0) c_2^*(0)] = 0. \tag{71}
\]

For initial state $C(0) = [\sqrt{3}/2, i/2]^T$ which does not satisfy (71), we have $S_d(0) = 0.562$. If the entropy is desired to increase to $S_d(T) = 0.6$ at time $T = 0.01$, the controller (51) can be calculated as $U(0) = 3.875$ or $-89.373$. Simulations of the entropy for system (69) with initial state $C(0) = [\sqrt{3}/2, i/2]^T$ under controller $U(0) = 3.785$ and $-89.373$ are shown in Figure 3.

From Figure 3 we can see that both controllers can achieve the goal. While $U(0) = -89.373$ can make the probability change very fast. This does not satisfy the premise of Theorem 1, thus the entropy cannot be accurately approximated. From (69) we can see when $U(0) = 0$, there will be no change in the probability distribution and the entropy. Since larger $|U(0)|$ leads to faster entropy change with oscillation, we just choose the controller with small modulus. Hence, in (51), when $DN > 0$ we choose plus; otherwise we choose minus. For $S_d(T) = 0.6$ and 0.5, when $T = 0.01, 0.001, 0.0001$, and 0.000001, the simulations are shown in Figure 4.

We can see the entropy can be driven to its destination at any prespecified time, which can be accomplished very quickly in one step. When the entropy has reached its target, from (23), we know that we can just apply $U(t) = 0$ to maintain the entropy unchanged for diagonal $A$. Here, the change of entropy in one step cannot be very large because Theorem 1 only holds for small change of the probability. In Section 6.2, we will show that multiple step tracking can be used to deal with large entropy change.

For initial state $C(0) = [\sqrt{3}/2, i/2]^T$, which satisfies (71), the entropy cannot be reduced in very small time $T$ with constant $U(0)$. This can be seen in Figure 5 which shows the change of entropy with respect to $S_d(0)$ at $T = 0.01$ under different $U(0)$.

From Figure 5, we can see that, no matter how large $U(0)$ is, the entropy at $T = 0.01$ is almost always larger than $S_d(0)$ except when $U(0) = -155$ and $-470$. The evolutions of the entropy under $U(0) = -155$ and $-470$ are shown in Figure 6.

From Figure 6, we can find that the entropy cannot be reduced at the beginning, but can be reduced later, which coincides with Theorem 4.

6.2. Simulation on a Three-Level System. Consider the following system:
\[
\begin{bmatrix}
c_1(t) \\
c_2(t) \\
c_3(t)
\end{bmatrix} = \begin{bmatrix} i & -i & 0 \\ -i & 0 & 0 \\ 0 & 0 & -i \end{bmatrix} U(t) \begin{bmatrix} c_1(t) \\
c_2(t) \\
c_3(t)
\end{bmatrix}. \tag{72}
\]
Since $DM = -T^2[|c_1(0)|^2 \ln |c_3(0)|^2 + |c_3(0)|^2 \ln |c_1(0)|^2] > 0$, we should always use (51) to calculate $U(0)$. The conditions under which the entropy cannot be reduced are as follows:

\[
DR[AC(0) \circ C^*(0)] = \mathfrak{F}[c_1(0) c_2^*(0)] \ln \frac{|c_1(0)|^2}{|c_2(0)|^2} \geq 0,
\]

\[
DR[BC(0) \circ C^*(0)] = \mathfrak{F}[c_1(0) c_3^*(0)] \ln \frac{|c_1(0)|^2}{|c_3(0)|^2} = 0.
\]

Assuming $C(0) = [\sqrt{6}/6, \sqrt{3}/3, \sqrt{2}/2]^T$, which does not satisfy the conditions, we have $S_d(0) = 1.011$. In seven steps, we expect that the entropy changes as follows: (a) increases to 1.05; (b) remains unchanged; (c) increases to 1.1; (d) remains unchanged; (e) decreases to 1.05; (f) increases to 1.1; (g) remains unchanged. The controller can be calculated as follows, where $1(t-t_0)$ denotes the unit step function starting from $t_0$.

Consider the following:

\[
U(t) = 5.582 - 4.385 \cdot 1(t - 0.01) + 7.603 \cdot 1(t - 0.02) - 3.926 \cdot 1(t - 0.03) - 14.667 \cdot 1(t - 0.04) + 17.137 \cdot 1(t - 0.05) - 1.452 \cdot 1(t - 0.06).
\]

The evolutions of the entropy and the quantum states are shown in Figure 7.

In order to overcome the delays, we can divide one step into halves and use predictions, which can be shown in Figure 8.

The time interval $(0.02, 0.03)$ is divided into two steps, and for each step the controller is calculated separately. At times 0.045 and 0.055 we use half step predictions which can lead to more accurate control. The improved controller is as follows:

\[
U(t) = 5.582 - 4.385 \cdot 1(t - 0.01) + 8.204 \cdot 1(t - 0.02) + 4.153 \cdot 1(t - 0.025) - 9.645 \cdot 1(t - 0.03) - 17.717 \cdot 1(t - 0.04) + 30.549 \cdot 1(t - 0.05) - 13.287 \cdot 1(t - 0.06).
\]

The simulations are shown in Figure 9.

7. Conclusion

This paper proposes a new quantum control method which controls the Shannon entropy of quantum systems. Simulation examples evidenced the effectiveness of the method. A strength of our method is that it provides a direct control algorithm for discrete quantum entropy, rather than the indirect one via PDF control. Our method provides a universal tool for entropy control, which can also contribute to classical information theory. Some immediate extensions of the method include quantum sliding-mode control and coherent control. The extension of the methods to the mixed state case deserves our future research. The applications in correlation energy and biological control are also of keen interests and currently being pursued.

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References


Research Article

Hybrid Impulsive Control for Closed Quantum Systems

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The state transfer problem of a class of nonideal quantum systems is investigated. It is known that traditional Lyapunov methods may fail to guarantee convergence for the non-ideal case. Hence, a hybrid impulsive control is proposed to accomplish a more accurate convergence. In particular, the largest invariant sets are explicitly characterized, and the convergence of quantum impulsive control systems is analyzed accordingly. Numerical simulation is also presented to demonstrate the improvement of the control performance.

1. Introduction

One of major concerns in quantum control is how to steer quantum states to a desired target state precisely and efficiently. A solution to this quantum state transfer problem will help us to advance some promising applications such as quantum computation and quantum chemistry. The main difficulty in quantum control is due to the limitations on the application of observation and feedback in quantum systems. Open-loop control has therefore been a commonly adopted approach in quantum control, where recorded control signals obtained from numerical simulations are implemented to real quantum systems. Among existing open-loop control design methods, the Lyapunov method could be the most popular one and has been tested in real applications [1–6]. Despite great advances have been made in Lyapunov methods, they may fail to achieve the control goal if the internal Hamiltonian is not strong regular [7]. This nonideal case means that distances between the eigenvalues of the internal Hamiltonian are not distinct. It is worth pointing out that this nonideal case does exist in many practical quantum systems such as coupled spin systems and harmonic oscillator systems [3, 4].

In particular, this paper will study the state transfer for closed quantum systems modeled as the following Schrödinger equation:

\[ i \left| \dot{\psi}(t) \right> = H_0 \left| \psi(t) \right> , \]

where \( H_0 \) is the internal Hamiltonian. For quantum systems, the control is implemented to the system through electromagnetic fields. Our basic problem is to transfer a quantum state from an initial state to a desired target state. The difficulty for the Lyapunov control of nonideal quantum system mainly comes from the fact that the system could be driven to undesired limit points in the invariant set. There exist a few results in the recent literature handling such a nonideal case. In [7], the complete controllability of the quantum systems with twofold degeneracy was investigated, and the basic idea is to apply a weak constant field to eliminate the degeneracy. In [4], the implicit Lyapunov method was used to deal with such a nonideal case. However, it is difficult to characterize invariant sets which are critical for the following convergence analysis. Therefore, we propose a new hybrid impulsive control strategy for closed quantum systems under the nonideal case. Nowadays, the impulsive control has proved to be an effective method to accomplish...
The basic idea of the hybrid impulsive control is to divide the control into a piecewise continuous open-loop coherent control $u_i(t)$ and an impulsive control $u_s$, $u_1(t)$ design is similar to the traditional Lyapunov control which drives states to invariant sets. Specifically, the system under the piecewise continuous control can be described by

$$i |\dot{\psi}(t)\rangle = \left[ H_0 + \sum_{l=1}^{r} H_l u_{jl}(t) \right] |\psi(t)\rangle, \quad t \neq t_k,$$

where $H_0$ is the control Hamiltonian and $u_{jl}(t)$ is real-valued control function ($l \in J = \{1, 2, \ldots, r\}$). The continuous-time coherent control $u_j(t)$ is implemented through the control Hamiltonians $H_l$ when $t \neq t_k$. Due to the nonideal quantum system, this control cannot guarantee the convergence to the desired target state. After a certain instant $t_k$, the controlled state would sufficiently approach an undesired limit point. Hence, the control could fail to drive the system state. Then we need to “kick” the state out of undesired limit point and drive it re-converge to new, hopefully desired, state. At $t = t_k$, the piecewise continuous control $u_j(t)$ is switched off, and the “kicking” effect is accomplished by the impulsive control $u_0(t)$, by which the controlled system at the instant $t_k$ becomes

$$i |\dot{\psi}(t)\rangle = \left[ H_0 + \overline{B}_k \delta (s - t_k) \right] |\psi(t)\rangle, \quad t \neq t_k,$$

where the introduced Hermitian operator $\overline{B}_k$ is the impulsive control Hamiltonian to be designed, $\delta(\cdot)$ is the Dirac impulse function with $u_0(t) = 0, t \neq t_k$, and $t_k$ is the impulsive instant at which the impulsive control is implemented, satisfying $\lim_{k \to \infty} t_k = \infty$. With the impulsive control $u_0(t)$, the state satisfies $|\psi(t_k + h)\rangle = e^{-i \int_{t_k}^{t_k+h} [H_0 + \overline{B}_k \delta (s - t_k)] dt} |\psi(t_k)\rangle$, for sufficiently small $h > 0$. As $h \to 0^+$, we have $\lim_{h \to 0^+} |\psi(t_k + h)\rangle = |\psi(t_k^+)\rangle = e^{-i \int_{t_k}^{t_k^+} H_1 dt} |\psi(t_k)\rangle$ and define $|\psi(t_k^-)\rangle = |\psi(t_k)\rangle = \lim_{h \to 0^-} |\psi(t_k - h)\rangle$. In the control process, in order to keep the coherence of the controlled state, the proposed control strategy is the open-loop coherent control.

In practical implementations, the $\delta$ function in the impulsive control can be substituted with pulses of finite duration if the duration is sufficiently short compared with the time scale of quantum systems [13]. In recent years, the impulsive control idea has been used in the control of open quantum systems to suppress decoherence, for example, bang-bang pulses [13–18], and the minimal time control of spin systems [19, 20]. It is realized by a sequence of unitary operations, characteristic of instantaneous pulses. The feasibility of this impulsive control was supported by physical experiments; see [14–17] and the references therein. The so-called hard pulses in NMR are analogous to this picture.

With this understanding, this paper will focus on the development of hybrid impulsive control design itself to achieve more accurate convergence under the nonideal cases. Moreover, the invariant set of the controlled system is characterized explicitly, which is shown to be strictly smaller than that obtained using classical Lyapunov methods.

The convergence analysis is then obtained via an extending LaSalle invariance principle for impulsive systems in [21]. Simulation studies show improved control performance.

The rest of this paper is organized as follows. In Section 2, we design the hybrid impulsive control for nonideal systems by the Lyapunov function based on the state distance. Properties of the controlled system are discussed, and the convergence is analyzed by explicit characterization of the LaSalle invariant set. In Section 3, using the Lyapunov function based on the state error, the hybrid impulsive control of quantum systems is investigated. Section 4 includes numerical simulation to demonstrate the effectiveness and advantage of the proposed methods. Finally, some conclusions are drawn in Section 5.

2. Hybrid Impulsive Control Based on the State Distance

In practice, we do not have much freedom to choose the control Hamiltonian due to the structure limitations of the control fields [3, 4]. The impulsive control Hamiltonian cannot be chosen arbitrarily to achieve the state transfer instantaneously. Thus in this paper, $H_1$ is fixed and assumed to be known beforehand. Denote $B_k = e^{-i \beta_k}$, which is unitary. With the hybrid impulsive control fields $u(t)$, system (1) becomes a closed quantum impulsive control system as follows:

$$i |\dot{\psi}(t)\rangle = \left[ H_0 + \sum_{l=1}^{r} H_l u_{jl}(t) \right] |\psi(t)\rangle, \quad t \neq t_k,$$

$$|\psi(t_k^-)\rangle = B_k |\psi(t_k)\rangle.$$
where $K_j > 0$ is the control gain and the function $f_i(\cdot)$ passes through the origin of plane $x_i - y_i$ monotonically satisfying $f_i(x_i)x_i \geq 0$ with $x_i = \mathfrak{F}(|\psi_j|H^iI\vert\psi\rangle)$. To avoid the confusion, we define $\langle\psi_j|\psi\rangle = 0$ if $|\psi\rangle = 0$. In addition, the impulsive control matrix $B_k$ should be chosen to satisfy $\Delta V_i(t_k) \leq 0$; that is,

$$B_k^* \rho_j B_k - \rho_j \geq 0,$$

(7)

where $\rho_j = |\psi_j\rangle \langle \psi_j|$ is the density matrix of target state $|\psi_j\rangle$.

Inequality (7) holds at least for the unitary matrix $B_k$ which commutes with $\rho_j$. The control law satisfying (6) and (7) is the designed control law. In the following, the properties of system (4) will be studied to show that $u(t)$ can make the system leave the initial state even if $|\psi(0)\rangle$ is an eigenstate of $H_0$.

**Lemma 1.** For control law (6) and (7), if the initial state is an eigenstate of $H_0$ with $H_0|\psi(0)\rangle = \lambda_0|\psi(0)\rangle$ and $\langle \psi(0)|\psi\rangle = 0$, then the following conclusions hold:

(i) if there exists $l \in J$ such that $\mathfrak{F}(\psi_j|H_l\vert\psi\rangle) \neq 0$, then $\langle \psi(t)|\psi\rangle \neq 0 (t > 0)$;

(ii) if $\mathfrak{F}(\psi_j|H_l\vert\psi\rangle) = 0$, for all $l \in J$, and there exists $l \in J$ such that $\{\mathfrak{F}(\psi_j|H_l\vert\psi\rangle) \neq 0$ and $\lambda_0 \neq 0$, then $\langle \psi(t)|\psi\rangle \neq 0, t > t^*$, where $t^*$ is sufficiently small; otherwise, the designed control fields cannot achieve the state steering of the closed-loop system.

**Proof.** (i) For a sufficiently small $dt$, as $t \neq t_k$, we have $i\langle \psi(t)| \psi(t)\rangle = i \lim_{dt \to 0} \frac{|\psi(dt)| - |\psi(0)|}{dt} = H|\psi(0)\rangle$; that is, as $dt \to 0$, $|\psi(dt)| = (I - iHdt)|\psi(0)\rangle$. Since $\langle \psi(0)|\psi\rangle = 0$, the inequality $\langle \psi(f)|dt\psi\rangle \neq 0$ is equivalent to $\sum_{l=1}^{J} u_{ij}(\psi_j\langle H_l|\psi\rangle) = \sum_{l=1}^{J} u_{ij}\mathfrak{F}(\psi_j|H_l\vert\psi\rangle) + \mathfrak{F}(\psi_j|H_l\vert\psi\rangle) \neq 0$. By (6), we have $u_{ij}\mathfrak{F}(\psi_j|H_l\vert\psi\rangle) \geq 0$, for all $l \in J$. It follows from the assumption in case (i) that there exists $l \in J$ such that $u_{ij}\mathfrak{F}(\psi_j|H_l\vert\psi\rangle) > 0$, and consequently, $\langle \psi(t)|dt\psi\rangle \neq 0$. Since $V_1 \leq 0$, we obtain that $\langle \psi(t)|\psi\rangle \neq 0, t \in (0, t_1)$. By (7) we have $\langle \psi_j|dt\psi\rangle|_{t=t_1} \geq 0$. Hence, we obtain that $\langle \psi(t)|\psi\rangle \neq 0, t > 0$.

(ii) Initially, the system evolves freely because $u_{ij}(0) = 0, l \in J$. For a sufficiently small $t^* < t_1$, one can obtain that $|\psi(t^*)\rangle = e^{-Hdt^*}|\psi(0)\rangle = e^{-Ht^*}|\psi(0)\rangle$. Moreover, as $dt \to 0$, we have $\langle \psi|\psi(t^* + dt)\rangle = \langle \psi|(I - iHdt)|\psi(t^*)\rangle = dt\langle \psi| - \cos(\lambda_0 t^*) - i\sin(\lambda_0 t^*)\sum_{j=1}^{J}\langle \psi_j|H_jdt|\psi\rangle \rangle \neq 0$. Noticing that there exists $l \in J$ such that $\langle \psi_j|H_l|\psi\rangle \neq 0$, we have $\langle \psi|\psi(t^*)\rangle = K_i\mathfrak{F}(e^{-iHdt^*}|\psi_j|H_l\vert\psi\rangle) = K_i\mathfrak{F}[-\sin(\lambda_0 t^*)\langle \psi_j|H_j\vert\psi\rangle \rangle \neq 0$. Similar to the discussion in case (i), we obtain that $\langle \psi_j|dt\psi\rangle \neq 0$, and then $\langle \psi(t)|\psi\rangle \neq 0, t > t^*$. This completes the proof.

For the characterization of invariant sets, properties of the states such that $V_1 = 0$ are studied. Since the proof is similar to that of Proposition 4 in [1], we omit it here.

**Lemma 2.** If $\langle \psi_j|\psi\rangle = 0$ and the conditions (i) or (ii) in Lemma 1 hold, the following conclusions are equivalent:

(i) $V_i(t) = 0, t \neq t_k$,

(ii) $\langle \psi(t)|\psi\rangle = H_0|\psi(t)\rangle, t \neq t_k$,

(iii) there exists $\lambda_1 \in \mathbb{R}$ such that $\langle \psi_j|(\lambda_1 I - H_j)|\psi(t)\rangle = 0, t \neq t_k, l \in J$.

Lemma 2 only characterizes the states guaranteeing that $V_i = 0$ at specific instants. We need to characterize the states from which the system trajectories stay in the set $V_i = 0$ and $\Delta V_i = 0$. We first present the extensive LaSalle invariance principle for impulsive systems in [21].

**Lemma 3.** Consider the following differential impulsive system on an open set $\mathcal{D}$:

$$\dot{x}(t) = f_c(x(t)), \quad x(0) = x_0, t \neq t_k,$$

$$\Delta x(t) = f_d(x(t)), \quad t = t_k.$$

If there exists a continuous function $V$ such that $V^*(x)f_c(x) \leq 0, t \neq t_k$ and $\Delta V(t_k) \leq 0$, then $x(t) \rightarrow M$ as $t \rightarrow \infty$, where $M$ is the largest invariant set contained in $\mathcal{D} \equiv \{x : V^*(x)f_c(x) = 0\} \cap \{x : \Delta V(x) = 0\}$.

**2.2. Convergence Analysis.** The following theorem presents the characterization of the invariant set for the nonideal systems under the hybrid impulsive control, by which the invariant set is smaller compared with that obtained by the conventional Lyapunov method. In the following, the unitary matrix $B_k$ is designed such that it commutes with $H_0, k \in Z^*$. 

**Theorem 4.** Consider system (4) with the hybrid impulsive control satisfying (6) and (7). The largest invariant set is given by $G = \mathbb{S}^{2n-1} \cap E_1 \cap E_2$ with $E_1 = \{\psi : |\psi\rangle \in M_k^l\}$, for all $l \in J, k = 1, 2, \ldots$, $E_2 = \{\psi : |\psi\rangle \in N_k, k = 1, 2, \ldots\}$,

$$M_k^l := \{\psi : \mathfrak{F}(\psi_j|\psi\rangle \langle \psi_j|X_l^k|\psi\rangle = 0, s_l = 1, 2, \ldots, m_l\},$$

$$N_k := \left\{\psi : \langle \psi|\frac{1}{\sqrt{\prod_{j=1}^{k-1} B_j}}|\psi_j\rangle \langle \psi_j|X_l^k \prod_{j=1}^{k-1} B_j |\psi\rangle \rangle = 0, s_l = 1, 2, \ldots, m_l\right\}, \quad k \geq 2,$$

(9)

where $X_l^1, X_l^2, \ldots, X_l^{m_l}$ constitute the basis of the set $\{(i)^{l}(H_0^{(i)}), H_0^{(i)}, l = 0, 1, 2, \ldots, l \in J\}$. Hence, system (4) converges to $G$ under the hybrid impulsive control.
Proof. When \( t = t_0 \), from (6), we obtain that
\[
\mathcal{V}_1(t_0) = 0 \iff \left( \left\langle \psi(t_0) \right| \left| \psi_f \right> \right) \\
\times \mathfrak{S} \left[ e^{i\left\langle \psi(t_0) \right| \psi_f> \left( \left| \psi_f > H_j \left| \psi(t_0) \right> \right) \right] = 0, \quad l \in J \\
\mathfrak{S} \left( \left\langle \psi(t_0) \right| \left| \psi_f \right> \right) = 0.
\]
(10)

The main idea of the proof is sketched as follows. The interval \([t_{k-1}, t_k]\) is divided into \( n_k \) sufficiently small intervals with duration \( dt \). We apply the Taylor expansion on the system state and omit the high order terms of \( dt \). By Lemma 2, the requirements \( \mathcal{V}_1(t) = 0 \) \((t \neq t_k)\) and \( \Delta V_1(t_k) = 0 \) for the whole system trajectory will be transformed to the conditions on the initial state. By the Taylor expansion and commutativity between \( H_0 \) and \( B_k \), it yields that
\[
\mathcal{V}_1(t_0 + dt) = 0 \\
\mathfrak{S} \left( \left\langle \psi(t_0 + dt) \right| \left| \psi_f \right> \right) = 0 \\
\mathfrak{S} \left( \left\langle \psi(t_0) \right| \left( 1 + iH_0 dt \right) \left| \psi_f \right> \right) \\
\times \left( \left| \psi_f > [H_0, H_j] \left| \psi(t_0) \right> \right) = 0, \quad l \in J \\
\mathfrak{S} \left( \left\langle \psi(t_0) \right| \left| \psi_f \right> \right) = 0.
\]
(11)

At \( t = t_k + dt \), the free evolution of \( |\psi(t)\rangle \) is given by
\[
|\psi(t_k + dt)\rangle = \left( 1 - iH_0 dt \right) |\psi(t_k)\rangle \\
= B_k \left( 1 - iH_0 dt \right) |\psi(t_k)\rangle, \quad k = 1, 2, \ldots.
\]
(12)

Similar to the previous deduction, it follows from (11) and (12) that
\[
\mathcal{V}_1(t_k + dt) = 0 \\
\mathfrak{S} \left( \left\langle \psi(t_k + dt) \right| \left| \psi_f \right> \right) = 0 \\
\mathfrak{S} \left( \left\langle \psi(t_k) \right| \left| \psi_f \right> \right) \\
\times \left( \left| \psi_f > [H_0, H_j] \left| \psi(t_k) \right> \right) = 0, \quad s = 0, 1
\]

Consequently, it can be obtained that
\[
D^{-1} \mathcal{V}_1(t_k) = 0 \\
\mathfrak{S} \left( \left\langle \psi(t_k) \right| \left( \prod_{j=1}^{k-1} B_j \right) \left| \psi_f \right> \right) \\
\times \left( \left| \psi_f > [H_0^{(s)}, H_j] \prod_{j=k-1}^{1} B_j \left| \psi(t_k) \right> \right) = 0,
\]
(14)

where \( s = 0, 1, \ldots, \sum_{j=1}^{k} n_j \). Noticing that the set \{\langle \psi \rangle | \left[ H_0^{(s)}, H_j \right], s = 0, 1, \ldots, \sum_{j=1}^{k} n_j \}, l \in J \) has finite dimension, we denote its basis to be \( X_1^1, X_1^2, \ldots, X_1^{m_1} \), \( l \in J \). Since the division of the interval \([t_{k-1}, t_k]\) is random, (14) can be rewritten as
\[
D^{-1} \mathcal{V}_1(t_k) = 0 \\
\mathfrak{S} \left( \left| \psi(t_k) \right| \left( \prod_{j=1}^{k-1} B_j \right) \left| \psi_f \right> \right) \\
\times \left( \left| \psi_f > \prod_{j=k-1}^{1} B_j \left| \psi(t_k) \right> \right) = 0,
\]
(15)

For convenience, the set of the states satisfying (15) is denoted as \( \mathcal{M}_k \) in (9), \( l \in J, k \geq 2 \).

In the following, we will discuss the conditions on the initial states from which the trajectories stay in the set \{\langle \psi \rangle : \Delta V_1(t_k) = 0, k = 1, 2, \ldots \}:
\[
\Delta V_1(t_1) = 0 \\
\mathfrak{S} \left( \left\langle \psi(t_1) \right| B_s^* \left| \psi_f \right> \right) \\
\times \left( \left| \psi_f > \prod_{j=1}^{1} B_j \left| \psi(t_1) \right> \right) = 0.
\]
achieve more accurate convergence under the nonideal case. This implies that the proposed hybrid impulsive control can reduce to Theorem 2 in [1]. For the nonideal case, it is clear that Corollary 5.

Let \( \omega = -\lambda_f \). We design the following control to ensure \( V_2(t) \leq 0, t \neq t_k \):

\[
\lambda_f + \omega = u_0 = K_0 f_0 \left( \mathfrak{H} (\psi_f | \psi) \right),
\]

\[
u_1 = K_1 f_1 \left( \mathfrak{H} (\psi_f | H_1 | \psi) \right),
\]

where \( K_1 > 0 \), and the function \( y_1 = f_1(\cdot) \) is defined as that in (6).

**Theorem 7.** Consider system (18) with control fields (7) and (20). The largest invariant set is given by \( K = F_1 \cap F_2 \cap S^{2n-1} \), where \( F_1 = \{ |\psi\rangle : |\psi\rangle \in U_k, k = 1, 2, \ldots \} \), \( F_2 = \{ |\psi\rangle : |\psi\rangle \in W_k, k = 1, 2, \ldots \} \), and \( U_k := \{ |\psi\rangle : \mathfrak{R} (\psi_f | X^s | \psi) = 0, s = 1, \ldots, m_1 \} \), \( W_k := \{ |\psi\rangle : \mathfrak{R} (\psi_f | \psi) = 0 \} \) \( k \geq 1 \),

\[
U_k := \left\{ |\psi\rangle : \mathfrak{H} (\psi_f | X^s \prod_{j=k-1}^1 B_j | \psi) = 0, s = 1, \ldots, m_1 \right\},
\]

\[
W_k := \left\{ |\psi\rangle : \mathfrak{R} (\psi_f | \psi) = 0 \right\}, \quad k \geq 1,
\]

where \( X^1, X^2, \ldots, X^{m_1} \) are the basis of the set \( \{I, (i)^{s} [H_0^{(s)}, H_1] \}, s = 0, 1, 2, \ldots \}. Therefore, system (18) converges to \( K \) with the hybrid impulsive control satisfying (7) and (20).

**Proof.** Let \( \omega = -\lambda_f \). When the system satisfies \( V_2 = 0 \), that is, \( u_1 = 0 \), the evolution of system (18) becomes

\[
i |\psi (t)\rangle = \left( H_0 - \lambda_f I \right) |\psi (t)\rangle, \quad t \neq t_k,
\]

\[
|\psi (t_k)\rangle = B_k |\psi (t_k)\rangle.
\]

**Corollary 5.** Consider system (4) with control field (6) without the impulsive control, that is, \( B_k = I, k = 1, 2, \ldots \). The largest invariant set is \( E \cap \mathcal{S}^{2n-1} \), where \( E = \{ |\psi\rangle : |\psi\rangle \in M_{k}, k \in \mathbb{N} \} \). We denote the set of the states guaranteeing (17) to be \( N_k \) in (9).

In conclusion, all the states which stay in the intersection \( E_1 \cap E_2 \) constitute the largest invariant set of system (4). By Lemma 3, we complete the proof.

It should be noticed that the basis of the set \( \{ (i)^{s} [H_0^{(s)}, H_1] \}, s = 0, 1, 2, \ldots, n \} \) can be obtained in finite steps, \( l \in J \). If the first \( n^2 \) elements in the set are linearly independent, then they constitute the basis. \( [H_0^{(n+1)}, H_1] \) can be represented by the first \( s \) elements, it is easy to obtain that \( [H_0^{(n)}, H_1] \) can be represented by the linear combination of \( H_1, [H_0, H_1], \ldots, [H_0^{(s)}, H_1] \), for all \( k > s \).

**Remark 6.** If \( H_0 \) is strong regular, then the result in Corollary 5 reduces to Theorem 2 in [1]. For the nonideal case, it is clear that \( G \subset E \). From the viewpoint of physics, this implies that the proposed hybrid impulsive control can achieve more accurate convergence under the nonideal case. In general, the matrix \( B_k \) can be chosen to guarantee that \( E_1 \) and \( E_2 \) contain finite sets \( M_{k} \) and \( N_k \). It can be found that the invariant set \( G \) depends on the choice of impulsive control matrix \( B_k \). The optimal determination of \( B_k \) and impulsive instants \( t_k \) to minimize the invariant set are under study.

**3. Hybrid Impulsive Control Based on the State Error**

It is known that different Lyapunov functions may have different control effects. The relations among them were studied in our previous work [4]. In this section, we consider the hybrid impulsive control of quantum systems based on the state error between the controlled state and the goal state. Let \( V_2 (\psi (t)) = V_2 (t) = (1/2) \langle \psi (t) - \psi_f | \psi (t) - \psi_f \rangle = 1 - \mathfrak{R} (\psi_f | \psi) \). Similar to the hybrid control design in Section 1,
It follows from (22) that
\[
|\psi (t_{k-1} + dt)\rangle = |\psi (t_{k-1})\rangle + |\psi (t_{k-1})\rangle dt = \left[ I - i \left( H_0 - \lambda_f I \right) dt \right] |\psi (t_{k-1})\rangle.
\] (23)

From (20), we obtain the following relation:
\[
V_2 (t_0) = 0 \iff \mathcal{S} \left( \left( \langle \psi_f | H_1 | \psi (t_0) \rangle \right) = 0, \right.
\]
\[
\mathcal{S} \left( \left( \langle \psi_f | H_0 | \psi (t_0) \rangle \right) = 0. \right)
\] (24)

Similarly, we divide the interval \([t_{k-1}, t_k]\) into \(n_k\) sufficiently small intervals. From (22)–(24), we have \(D^- V_2(t_k) = 0 \iff \mathcal{S} \left( i^{n_k} \langle \psi_f | [H_0^{(n_k)}, H_1] | \psi (t_0) \rangle \right) = 0. \) According to the similar method in the proof of Theorem 4, when \(t = t_k\), it yields that
\[
D^- V_2(t_k) = 0
\]
\[
\iff \mathcal{S} \left( \left( \langle \psi_f | H_1 | \psi (t_0) \rangle \right) = 0, \right.
\]
\[
\mathcal{S} \left( \left( \langle \psi_f | H_0 | \psi (t_0) \rangle \right) = 0. \right)
\] (25)

where \(s = 0, \ldots, \sum_{i=1}^{k} n_i\). Denote the basis of the set \(\{ i, i^2 \langle H_0^{(i)}, H_1 \rangle, s = 0, 1, \ldots, \sum_{i=1}^{k} n_i \} \) to be \(X^1, X^2, \ldots, X^{m_1}\). Equation (25) can be rewritten as \(D^- V_2(t_k) = 0 \iff \mathcal{S} \langle \psi_f | X^s \prod_{j=k-1}^{1} B_j | \psi (t_0) \rangle = 0, s = 1, 2, \ldots, m_1\). This equality is denoted as \(V_2(t_k) \) in (21).

Next, we characterize the initial states from which the system trajectories stay in \(|\psi\rangle : \Delta V_2(t_k) = 0, k = 1, 2, \ldots \). From the definition of \(V_2\), we have \(\Delta V_2(t_1) = \mathcal{R} \langle \psi_f | \psi (t_1^*) \rangle - \mathcal{R} \langle \psi_f | \psi (t_1) \rangle = \mathcal{R} \langle \psi_f | B_1 | \psi (t_1) \rangle - \mathcal{R} \langle \psi_f | \psi (t_1) \rangle \). The following relations can be obtained:
\[
\Delta V_2(t_1) = 0
\]
\[
\iff \mathcal{R} \langle \psi_f | \psi (t_1) \rangle - \mathcal{R} \langle \psi_f | B_1 | \psi (t_1) \rangle = 0
\]
\[
\iff \mathcal{R} \langle \psi_f | (I - B_1) \left[ I - i \left( H_0 - \lambda_f I \right) dt \right] \times | \psi (t_1 - dt) \rangle = 0 \]
\[
\iff \mathcal{R} \langle \psi_f | \psi (t_0) \rangle - \mathcal{R} \langle \psi_f | B_1 | \psi (t_0) \rangle = 0.
\] (26)

By similar deduction, it yields that \(\Delta V_2(t_k) = 0 \iff \mathcal{R} \langle \psi_f | \psi (t_k) \rangle - \mathcal{R} \langle \psi_f | \prod_{j=k-1}^{1} B_j | \psi (t_0) \rangle = 0\), which can be denoted as \(W_k(t_0)\) in (21).

In conclusion, all the states which remain in the intersection \(F_1 \cap F_2\) constitute the largest invariant set of controlled system (18). By Lemma 3, the proof is completed. \(\Box\)

Similar to the discussion in Corollary 5, Theorem 7 can be reduced to Theorem 8 in [1] if there is no impulsive control, and \(H_0\) is strong regular. We can see that our result reduces the invariant set for the nonideal case. This implies that the proposed hybrid impulsive control scheme can accomplish more accurate state transfer.

4. Numerical Simulation

Example 1. Consider the five-level system with the internal Hamiltonian and impulsive control Hamiltonian given by
\[H_0 = \text{diag}(1.0, 1.2, 2.0, 2.15)\] and \(B_k = \text{diag}(0, 0, -\pi, -\pi, 0)\), respectively. The unitary operation \(B_k = e^{-i\pi_b} = \text{diag}(1, 1, -1, -1, 1)\) can be realized by performing the planar rotation on system states. It can be found that the system is a nonideal system. The control Hamiltonians are given by
\[H_1 = \left( \begin{array}{cc} 0 & 0 i 0 0 i 0 \\ -i 0 0 & 0 0 -i 0 0 \\ 0 0 -i 0 & 0 i 0 0 \\ -i 0 0 & 0 0 -i 0 \end{array} \right), \quad H_2 = \left( \begin{array}{cc} 0 & 0 0 0 0 \\ 0 i 0 0 0 & 0 0 i 0 0 \end{array} \right).\]

Let the target state be \(|\psi_f\rangle = [0 0 1 0 0]^T\), let the initial state be \(|\psi_0\rangle = [0 1 0 0 0]^T\), and let the control state be \(|\psi\rangle = [c_1, c_2, \ldots, c_5]^T\). Take the control function to be \(f_i(x) = x, i = 1, 2\). Choose the impulsive instant to be \(t_k = 3k - 1, k \in \mathbb{Z}^+\) and \(K_1 = K_2 = 0.2\). Using the hybrid impulsive control based on the state distance, simple computation yields that the invariant set \(G = \{|3\}\) (without regard to the global phase), which implies that under the hybrid impulsive control the system converges to \(|\psi_f\rangle\). The populations of the controlled system are illustrated in Figure 1.

Now we compare performance of the hybrid impulsive control with that of classical Lyapunov control. If the impulsive control is not applied to the system, then the hybrid impulsive control is reduced to the classical Lyapunov control, by which the performance of the controlled system is shown in Figure 2. Hence, the proposed hybrid impulsive control improves the control performance.

Example 2. Consider the five-level system with the same internal Hamiltonian as the previous example. Let the target state and the initial state be \(|\psi_f\rangle = [0 0 0 0 1]^T\) and \(|\psi_0\rangle = [1 0 0 0 0]^T\), respectively, and the impulsive control Hamiltonian \(B_k = \text{diag}(-\pi, 0, 0, -\pi, 0)\). The unitary operation is chosen as \(B_k = e^{-i\pi_b} = \text{diag}(-1, 1, 1, -1, 1)\). The system is a nonideal system. The control Hamiltonian is given
Figure 2: The population of the system state by the Lyapunov control without impulsive control.

Figure 3: The population of the system state by the hybrid impulsive control based on the state error.

Figure 4: The population of the system state by the Lyapunov control without impulsive control.

Figure 5: The population of the system state by the implicit Lyapunov control in [4].

by $H_1 = \begin{pmatrix} 0 & i & 0 & i \\ -i & 0 & 0 & i \\ 0 & 0 & 0 & i \\ 0 & -i & 0 & 0 \end{pmatrix}$. Let the control function be $f_1(x) = x$, and $K_0 = 0.1$, $K_1 = 0.2$. Choose the impulsive instant as $t_k = 3k - 1$, $k \in \mathbb{Z}^+$. Using the hybrid impulsive control based on the state error, simple computation yields that the invariant set $K = \{|5\rangle\}$ (without regard to the global phase), which implies that under the hybrid impulsive control the system converges to $|\psi_f\rangle$. Simulation results are illustrated in Figure 3.

When the hybrid impulsive control is reduced to the classical Lyapunov control, the trajectory of the controlled system is plotted in Figure 4. Moreover, if the implicit Lyapunov control strategy in [4] is employed with the same parameters, it fails to drive the system, as illustrated in Figure 5. Therefore, the proposed hybrid impulsive control improves the control performance.

5. Conclusion

In this paper, the coherent hybrid impulsive control for closed quantum systems has been investigated for the nonideal case that $H_0$ is not strong regular. The dynamical properties of the resulted quantum impulsive control system have been discussed to facilitate the convergence analysis. Based on two kinds of Lyapunov functions, the largest invariant sets have been characterized explicitly. Consequently, more accurate convergence of the controlled system has been achieved by the extensive LaSalle invariance principle. Compared with some existing results, the improved control performance has been shown for the nonideal case. Since the practical implementation of impulsive control has been studied in known literature, we believe that it is feasible. The optimal determination of the impulsive control Hamiltonian and impulsive instants is worth to be explored in the future work.

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References


Research Article

Simulation of Quantum Dynamics Based on the Quantum Stochastic Differential Equation

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The quantum stochastic differential equation derived from the Lindblad form quantum master equation is investigated. The general formulation in terms of environment operators representing the quantum state diffusion is given. The numerical simulation algorithm of stochastic process of direct photodetection of a driven two-level system for the predictions of the dynamical behavior is proposed. The effectiveness and superiority of the algorithm are verified by the performance analysis of the accuracy and the computational cost in comparison with the classical Runge-Kutta algorithm.

1. Introduction

Since Nelson successfully described the kinematics law of the quantum fluctuations by the Itô equation [1] and the Schrödinger equation was derived from Newtonian mechanics; the stochastic interpretation of quantum mechanics was established, in which a diffusion process was used to analyze the quantum fluctuation instead of the wave function. Then, the stochastic mechanics has gradually drawn much attention with research fields ranging from atomic and optical physics to condensed matter physics and quantum information science [2]. It becomes clear that a deep understanding of the effects of environments on a quantum system such as the mechanisms of decoherence and the dynamics of entanglement in the framework of quantum open systems is both of fundamental interest in quantum foundation issues and of practical importance in quantum information sciences. Many scholars have made thorough research on the quantum diffusion movement based on the basic theory and achieved fruitful results. For example, the normative structure of the dynamics equation of the particle fluctuation and its stability analysis methods were determined, followed by the unified interpretation of the Brown motion and the basic equation of the quantum mechanics [3–5]. The quantum stochastic dynamics elaborated the organic link between the microscopic behavior and macroevolution of the system, by which the details of the system evolution from any initial state to the final state can be analyzed. It has been successfully applied to the proliferation of microscopic particles, the molecular motors, the quantum chaos, and so forth [6].

Though the deterministic differential equations of quantum stochastic mechanics are relatively complex, it can be seen that with the development of the computer technology [7], the evolution of a microsystem can be analyzed using the numerical simulation method [8–10]. The quantum trajectory method is a typical one. It can be used for a wide range of open quantum systems to solve the master equation by unraveling the density operator evolution into individual stochastic trajectories in Hilbert space [11]. Over the last twenty years the theory of quantum trajectories has been developed by many researchers for a variety of purposes, including modeling continuously monitored open systems, improving numerical calculation and investigating the problem of quantum measurement [12, 13].

In this paper, based on the quantum stochastic dynamics, the master equation describing the time evolution law of the quantum state and its reduced density operator are investigated, and the effect of nonunitary operators on the evolution of the system is analyzed. Then the quantum stochastic differential equation is established to describe the microkinetic characteristics of the system, and a numerical
iterative algorithm for the simulation of the system evolution is proposed. The practicality and advantages of the algorithm are verified by comparison with the classical Runge-Kutta numerical iterative algorithm, which is followed by further discussions on the convergence of the algorithm.

2. Methods

The quantum state diffusion theory replaces the deterministic evolution of the density operator $\rho$ representing an ensemble of open systems [14]

$$\dot{\rho} = -\frac{i}{\hbar} [H, \rho] + \sum_j \left( L_j \rho L_j^+ - \frac{1}{2} L_j^+ L_j \rho - \frac{1}{2} \rho L_j^+ L_j \right)$$

(1)

by a unique stochastic diffusion of a quantum state, representing an individual system of the ensemble in interaction with its environment. $H$ is the Hamiltonian, and $L_j$ are a set of environment operators which represent the collective effects of interaction with the environment.

However, for some complicated systems, it can be very difficult to get either the analytical or the numerical solution of (1). In that case, it is often advantageous to take alternative ways considering an unraveling of the master equation into individual quantum trajectories. Quantum state diffusion (QSD) is one of these unraveling techniques. The corresponding quantum state diffusion equation is a stochastic differential equation for the normalized state vector $|\psi\rangle$ representing the pure state of the system that evolves according to the QSD equation. The differential Itô form is [15]

$$d|\psi\rangle = -\frac{i}{\hbar} H |\psi\rangle dt + \sum_j \left( \langle L_j^+ \rangle L_j - \frac{1}{2} L_j^+ L_j - \frac{1}{2} \langle L_j^+ \rangle \langle L_j \rangle \right) |\psi\rangle dt + \sum_j (L_j - \langle L_j \rangle) |\psi\rangle d\xi_j,$$

(2)

where $\langle L_j \rangle$ are defined by

$$\langle L_j \rangle = \langle \psi | L_j | \psi \rangle.$$

(3)

In the QSD equation, the standard normalized terms $d\xi_j$ represent independent complex Wiener processes and satisfy the relations

$$E d\xi_j = 0, \quad E (d\xi_j, d\xi_{j'}) = \delta_{jj'} dt,$$

(4)

where $E(\cdot)$ denotes an ensemble average of the noise. QSD reproduces the master equation in the mean

$$E (|\psi\rangle \langle \psi |) = \rho.$$

(5)

That is to say, the reduced state of the system, $\rho$, is obtained as an ensemble average. And this is what is meant by an unraveling of the master equation. Expectation values for operators obey a similar relationship:

$$\langle \hat{O} \rangle = \text{Tr} \{ \hat{O}\rho \} = E (\langle \hat{O} \rangle_\psi).$$

(6)

The use of QSD as a practical algorithm to solve master equations has been widely investigated [16, 17]. This includes calculations of output spectra in quantum optics [18]. As a practical method of computation, QSD gains over the direct solution of the master equation, because of a basis of $N$ states, QSD needs a computer store with $N$ elements, and the time of computation is also proportional to $N$. For the direct solution these are proportional to $N^2$.

In this paper, we take advantage of the system simulation method to simulate the evolutionary behavior of the open quantum systems and thus calculate and analyze various physical properties of the ensemble of open quantum systems. However, noting that we cannot usually get the analytical solution of (2), an alternative way is to find the numerical solution of the system evolution and investigate various control algorithms and control strategies based on the simulation method, which is a powerful tool built on the systems science, system identification, control theory, and computer technology for the analysis and synthesis of complex systems, especially large-scale systems [19].

In the system simulation, we should pay attention to the problem that the physical description of the stochastic process is relied on the master equation in the Lindblad operator form. If we want to get the numerical solution, the Lindblad operator must be explicitly quantified. Fortunately, existing results have summarized various forms of decoherence Lindblad operator in open quantum systems for reference; a general form of (2) can be written as [20]

$$d\psi(t) = D_1 (\psi(t)) dt + D_2 (\psi(t)) dW(t)$$

(7)

in which $dW(t)$ is a Wiener incremental process and the random items characterizing the system decoherence are

$$D_1 = \left( \langle L^+ \rangle L - \frac{1}{2} L^+ L - \frac{1}{2} \langle L^+ \rangle \langle L \rangle \right) |\psi\rangle,$$

$$D_2 = (L - \langle L \rangle) |\psi\rangle.$$

(8)

(9)

According to the above system model, in the given interval $[0, t_f]$, a sample of realization can be generated by the following algorithm [20].

(1) At the initial time $t = 0$, the initial state of the process $\psi'(0)$ is determined by the initial distribution.

(2) It is assumed that at time $t$, the normalized state $\psi'(t)$ is reached through a quantum jump; then we set $\psi'(t) = \tilde{\psi}$.

(3) Determine a random waiting time $\tau$. This can be done, for example, by drawing a random number $\eta$ which is uniformly distributed over the interval $[0, 1]$ and by determining $\tau$ from the equation:

$$\eta = 1 - F(\tilde{\psi}, \tau) = \|e^{-i\tau H} \tilde{\psi}\|^2.$$
First we define the defect of the waiting time distribution \( q \) by the identity

\[
q = \lim_{\tau \to \infty} \left\| \exp \left( -i \hat{H} \psi \right) \right\|^2.
\] (11)

For \( \eta > q \), a unique solution can be obtained. If \( \eta \leq q \), we set \( \tau = \infty \) in which case there will be no further jumps. Within the time interval \([t, t+\tau]\) the realization follows the deterministic time evolution:

\[
\psi^\tau(t + s) = \frac{e^{-i\hat{H}s}}{\left\| e^{-i\hat{H}s} \psi \right\|} \psi(t), \quad 0 \leq s \leq \tau.
\] (12)

(4) At time \( t+\tau \) (if \( \tau \) is finite and \( t+\tau < t_f \)), one of the possible jumps labeled by the index \( i \) occurs according to

\[
d\psi(t) = -i \left( \hat{H} + \frac{1}{2} \sum_i \gamma_i \|L_i \psi(t)\|^2 \right) \psi(t) dt + \sum_i \left( L_i \psi(t) - \psi(t) \right) \|L_i \psi(t) - \psi(t)\| \, \psi(t) \, dN_i(t).
\] (13)

Then we select a specific jump of type \( i \) with probability

\[
P_i = \frac{\gamma_i \|L_i \psi^\tau(t + \tau)\|^2}{\sum \gamma_i \|L_i \psi^\tau(t + \tau)\|^2}.
\] (14)

And then we update the state of system as

\[
\psi(t) = \frac{L_i \psi^\tau(t + \tau)}{\|L_i \psi^\tau(t + \tau)\|}.
\] (15)

(5) Repeat steps (1) to (4) until the desired final time \( t_f \) is reached, which yields the realization \( \psi^\tau(t) \) over the whole time interval \([0, t_f]\). Once a sample of realizations \( \psi^r(t), r = 1, 2, 3, \ldots, R \), has been generated according to this algorithm, any statistical quantity can be estimated through an appropriate ensemble average.

According to the above framework, an iterative algorithm is described as follows:

\[
\psi_{k+1} = \psi_k + \frac{1}{2} \left( D_1(\psi_k) + D_1(\psi_k) \right) \Delta t + \frac{1}{4} \left( D_2(\psi_k) + D_2(\psi_k) + 2D_2(\psi_k) \right) \Delta W_k
\]

\[
+ \frac{1}{4} \left( D_2(\psi_k) - D_2(\psi_k) \right) \left\{ (\Delta W_k)^2 - \Delta t \right\} \Delta t^{-1/2},
\] (16)

where

\[
\psi_k = \psi_k + D_1(\psi_k) \Delta t + D_2(\psi_k) \Delta W_k,
\]

\[
\tilde{\psi}_k = \psi_k + D_1(\psi_k) \Delta t \pm D_2(\psi_k) \sqrt{\Delta t}.
\] (17)

3. Results and Discussion

We consider the process describing the direct photodetection of a driven two-level system, and the piecewise deterministic process is given by the following equation [21, 22]:

\[
d\psi(t) = -i \left( \hat{H} + \gamma \|L \psi(t)\|^2 \right) \psi(t) dt + \left( \frac{\sigma_+ \psi(t)}{\|\sigma_+ \psi(t)\|} - \psi(t) \right) dN(t).
\] (18)

The Poisson increments \( dN(t) \) satisfy

\[
\hat{H} = H - \frac{1}{2} \sum \gamma_i L_i^\dagger L_i,
\]

\[
dN(t)^2 = dN(t), \quad E[dN(t)] = \|\sigma_+ \psi(t)\|^2 dt.
\] (19)

The corresponding stochastic Schrödinger equation takes the form

\[
d\psi(t) = -iH_\perp \psi(t) dt + \frac{\gamma}{2} \left( \langle \sigma_- + \sigma_+ \rangle \psi - \sigma_- \sigma_+ \psi \right) dt + \sqrt{\gamma} \left( \sigma_- - \frac{1}{2} \langle \sigma_- + \sigma_+ \rangle \right) \psi(t) dW(t),
\] (20)

where

\[
H_\perp = -\frac{\Omega}{2} \langle \sigma_- + \sigma_+ \rangle.
\] (21)

In the numerical simulations, it is assumed that the atom is in its ground state \( |g\rangle \) and the probability of finding the atom in the excited state \( |e\rangle \) can be calculated as follows:

\[
\rho_{11}(t) = \langle e | \rho(t) | e \rangle.
\] (22)

From a sample of realizations this probability is estimated by determining the average

\[
\overline{M}_1 = \frac{1}{R} \sum_{r=1}^{R} \langle e \psi^r(t) \rangle^2.
\] (23)

An appropriate estimator for the corresponding statistical errors in the determination of \( \overline{M}_1 \) from a finite sample of size \( R \) is given by

\[
\hat{\sigma}_1^2 = \frac{1}{R(R-1)} \sum_{r=1}^{R} \left( \langle e \psi^r(t) \rangle^2 - \overline{M}_1 \right)^2.
\] (24)

According [21, 22], the analytical solution of the process is

\[
\rho_{11}(t) = \frac{\Omega^2}{\gamma_0^2 + 2\Omega^2} \left[ 1 - e^{-\gamma_0 t/4} \left\{ \cos \mu t + \frac{3\gamma_0}{4\mu} \sin \mu t \right\} \right],
\] (25)
Table 1: The estimated means of $|\langle e|\psi'(T)\rangle|^2$ minus the exact values obtained by the analytical solution of $\rho_{11}(t)$, that is, $|\langle e|\psi'(T)\rangle|^2 - \rho_{11}(t)$, for different step sizes $\Delta t$ and methods.

<table>
<thead>
<tr>
<th></th>
<th>0.01</th>
<th>0.02</th>
<th>0.05</th>
<th>0.10</th>
<th>0.15</th>
<th>0.20</th>
<th>0.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>The proposed algorithm</td>
<td>0.00012</td>
<td>0.00018</td>
<td>0.00015</td>
<td>0.00025</td>
<td>0.00021</td>
<td>0.00017</td>
<td>0.00021</td>
</tr>
<tr>
<td>Runge-Kutta</td>
<td>0.00026</td>
<td>0.00049</td>
<td>0.00070</td>
<td>0.00121</td>
<td>0.00142</td>
<td>0.00220</td>
<td>0.00311</td>
</tr>
</tbody>
</table>

Table 2: The normalized CPU time for different step sizes $\Delta t$ and methods.

<table>
<thead>
<tr>
<th></th>
<th>0.01</th>
<th>0.02</th>
<th>0.05</th>
<th>0.10</th>
<th>0.15</th>
<th>0.20</th>
<th>0.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>The proposed algorithm</td>
<td>0.153</td>
<td>0.108</td>
<td>0.081</td>
<td>0.061</td>
<td>0.050</td>
<td>0.038</td>
<td>0.007</td>
</tr>
<tr>
<td>Runge-Kutta</td>
<td>1</td>
<td>0.162</td>
<td>0.100</td>
<td>0.083</td>
<td>0.072</td>
<td>0.065</td>
<td>0.030</td>
</tr>
</tbody>
</table>

where

$$\mu = \sqrt{\Omega^2 - \left(\frac{\gamma}{4}\right)^2}.$$  \hfill (26)

Hence, it is possible to compare the numerical results with the analytical results.

3.1. Simulation Results. A sample of realizations for $\rho_{11}$ calculated from (20) is shown as the dashed line in Figure 1 with the following parameters: step size $\Delta t = 0.01$, $\Omega = 0.45$, and $\gamma = 0.3$, while the smooth line shows the analytical solution.

In order to discuss the performance of the algorithm, we introduced the classic Runge-Kutta iterative algorithm for generating the sample of realizations as follows [23]:

$$\psi_{k+1} = \psi_k + \frac{1}{6} \left\{ \psi_k^1 + 2\psi_k^2 + 2\psi_k^3 + \psi_k^4 \right\} \Delta t + D_2 \left( \psi_k \right) \Delta W_k,$$  \hfill (27)

where

$$\psi_k^1 = D_1 \left( \psi \left( k \right) \right),$$
$$\psi_k^2 = D_1 \left( \psi_k + \frac{1}{2} \Delta \psi_k \right),$$
$$\psi_k^3 = D_1 \left( \psi_k + \frac{1}{2} \Delta \psi_k^2 \right),$$
$$\psi_k^4 = D_1 \left( \psi_k + \Delta \psi_k^3 \right).$$  \hfill (28)

In this paper, the computer simulation platform is the Intel(R) Core (TM)2 Duo CPU E7500 @ 2.93 GHz under the Windows XP operating system with the numerical calculation software Matlab7. By selecting different simulation step sizes $\Delta t$, we can get set of results according to the corresponding $\Delta t$ with different algorithms:

1. the estimated means of $|\langle e|\psi'(T)\rangle|^2$ minus the exact values obtained by the analytical solution of $\rho_{11}(t)$ for different step sizes and methods, $|\langle e|\psi'(T)\rangle|^2 - \rho_{11}(t)$, as Table 1 shows,

2. the normalized CPU time versus the absolute error for the data points, as Table 2 shows.

As can be seen from Table 1, when the simulation step size is increased, there is little change in the errors in the proposed algorithm, while the errors using the Runge-Kutta method increase linearly. That is, in a certain step length range, the proposed iterative algorithm can generate more accurate approximation numerical solution than the Runge-Kutta algorithm in comparison to the analytical solution.

At the same time, we can draw a conclusion from Table 2: when obtaining a more accurate numerical solution using the proposed algorithm, the computational time is on the same order of magnitude as the Runge-Kutta method consumes. And it is not difficult to find that, when the step length is gradually reduced, accompanied by improving the accuracy, the computational time of the Runge-Kutta algorithm grows faster.

Taking the above two advantages comparing to the classical Runge-Kutta algorithm, the proposed algorithm can generate a more accurate sample of realizations while paying lower computational costs, which reflects the superiority and practicality of the proposed algorithm.

3.2. Convergence Analysis. Generally speaking, the smaller the step size $\Delta t$ is, the closer the numerical solution matches the true solution, and consequently the convergence seems to take place. We denote $X(t_k)$ as the true analytical solution and $X_k$ as the numerical approximation. Noting that $X(t_k)$ and $X_k$ are random variables, we can measure the difference using $E(X_k - X(t_k))$, where $E(\cdot)$ represents the expected value.
Then a method is said to have strong order of convergence equal to $\beta$ if there exists a constant $M$ such that

\[ E |X_k - X(t_k)| \leq M \Delta t^\beta \]  

(29)

for any fixed $t_k \equiv t_0 + k \Delta t \in [0, t_f]$ and $\Delta t$ sufficiently small.

The strong order of convergence (29) measures the rate at which the “mean of the error” decays as $\Delta t \to 0$. A less demanding alternative is to measure the rate of decay of the “error of the means.” This leads to the concept of weak convergence. A method is said to have weak order of convergence equal to $\beta$ if there exists a constant $M$ such that

\[ E_p (X_k) - E_p X(t_k) \leq M \Delta t^\beta \]  

(30)

for any fixed $t_k \equiv t_0 + k \Delta t \in [0, t_f]$ and $\Delta t$ sufficiently small [24].

According to the above theory, we consider a numerical algorithm to integrate (7) in the time period $[t_0, t_0 + T]$. Such an algorithm will generate a discrete time approximation realization $\psi_n$ for the exact process $\psi(t_k)$ at the given time $t_k = t_0 + k \Delta t$, where $k = 0, 1, \ldots, n = T/\Delta t$. Before our discussion, several conventions should be made as follows.

1. In this section, $\psi_n$ always represents a numerical approximation, while $\psi(t_k)$ stands for the exact process described by (7).

2. Similarly, we define the discrete time approximation of the density matrix as $\rho_k = E[|\psi_n\rangle\langle\psi_n|]$, whereas $\rho(t) = E[|\psi(t)\rangle\langle\psi(t)|]$ is the exact density matrix satisfying the Lindblad equation (9).

3. We always set a deterministic initial state $\psi_0 \equiv \psi(t_0)$.

In order to illustrate the numerical convergence of the algorithm, we will compare the Taylor expansion of the exact density matrix $\rho(t)$ which is given by (31) with the generated approximation $\rho_k$:

\[ \rho(t + \Delta t) = \rho(t) + \mathbf{L} \rho(t) \Delta t + \frac{1}{2} \mathbf{L}^2 \rho(t) \Delta t^2 + O(\Delta t^3). \]  

(31)

We compare the numerical simulation approximate obtained by the proposed algorithm to the true evolution $\rho(t)$. The single-step error of a certain numerical scheme may then be expressed through the difference

\[ \rho_1 - \rho(t_1) = O(\Delta t^\gamma) \]  

(32)

which means that the strategy reproduces the Taylor expansion of $\rho(t)$ including terms of order $\gamma - 1$ in $\Delta t$.

Thus, it is direct to prove that the integration over a finite time period $[t_n, t_0 + T]$ decreases the convergence order by one since $n = T/\Delta t$ time steps are needed to compute the density at time $t_n = t_0 + T$, that is,

\[ \rho_n - \rho(t_n) = O(\Delta t^\beta) \]  

(33)

with $\beta = \gamma - 1$. If (33) can be satisfied, the numerical strategy is defined to be a strategy of order $\beta$ [15]. It should be noted that (33) is a special case of weak convergence of order $\beta$ describing the degree of proximity of the probability distributions of $\psi_n$ and $\psi(t_n)$ which is a much weaker criterion comparing to strong convergence defined in (29). In actual applications, one tends to care about this weaker form of convergence especially when considering the approximation of functionals of the stochastic variable.

When investigating the stochastic differential equations and numerical simulation solution process, if the issues are related to the numerical simulation of the stochastic process, the evaluation criteria of the solutions convergence are usually defined as the numerical approximation curve. It must be sufficiently close to the real trace of the evolution. That is to say, the higher the convergence order is, the closer the distribution of the numerical solution is with the analytical solution of the distribution. So it requires that the probability distribution $\psi_n$ obtained by the simulation iterative algorithm is close enough to the probability distribution determined by the quantum master equation [24].

Performing the error analysis according to (16) one can find it converging with order $\beta = 2$ in contrast to the classical Runge-Kutta method with $\beta = 1$. Thus, it is really a higher-order strategy in the weaker convergence sense.

4. Conclusions

The decoherence of open quantum systems usually makes the system evolve from the initial pure state to mixed states (in some cases, may also be mixed state into a pure state). Being a powerful tool for investigating the open quantum systems, the quantum master equation can give a quantitative description of the transition, dissipation, and decoherence caused by the interaction between the closed system and the environment. Taking this as the starting point of our research, in order to obtain the evolution of the open quantum systems according to its dynamic characteristics, we used the system simulation method to get the numerical solution to the reduced density operator of a typical open quantum system. And its effectiveness and superiority were verified in comparison with the classical algorithm. Further research includes the control scheme [25, 26] for quantum manipulation based on the characteristics of quantum dynamics.

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References


Research Article

A Coherence Preservation Control Strategy in Cavity QED Based on Classical Quantum Feedback

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For eliminating the unexpected decoherence effect in cavity quantum electrodynamics (cavity QED), the transfer function of Rabi oscillation is derived theoretically using optical Bloch equations. In particular, the decoherence in cavity QED from the atomic spontaneous emission is especially considered. A feedback control strategy is proposed to preserve the coherence through Rabi oscillation stabilization. In the scheme, a classical quantum feedback channel for the quantum information acquisition is constructed via the quantum tomography technology, and a compensation system based on the root locus theory is put forward to suppress the atomic spontaneous emission and the associated decoherence. The simulation results have proved its effectiveness and superiority for the coherence preservation.

1. Introduction

The enormous potential of quantum information has caused the widespread concern in the scientific community and has become an important research focus. Among the implementation of hardware design for quantum computing such as cavity QED, ion trap, nuclear magnetic resonance, quantum dots, and superconducting systems [1], cavity QED is one of the most promising schemes because the basic interaction within cavity QED is the vacuum Rabi oscillation and the strong coupling of cavity field and atom allows atom-photon system to maintain good quantum coherence within the time scale of the kinetic characteristics. Therefore, a variety of entangled state preparation methods have been proposed based on cavity QED. Accordingly, the advantages of cavity QED have made it possible to construct decisive multiparticle entanglement in experiment using it [2, 3].

However, all the advantages in cavity QED depend on the coherence of the system. The loss of coherence in quantum mechanical superposition states limits the time for which quantum information remains useful. Similarly, it limits the distance over which quantum information can be transmitted [4]. Hence, decoherence is the major obstacle that hinders the processing of quantum information in various physical implementations [5]. The preservation of quantum coherence is of fundamental importance in the hardware implementation of quantum information. In cavity QED, the foundation of quantum information processing is the Rabi oscillation, an undamped oscillation process, which can be destroyed by the spontaneous emission of the atom. Thus, aiming at eliminating the decoherence effects in cavity QED, a classical feedback control strategy is presented based on the transfer function of the Rabi oscillation. A feedback channel is constructed through the quantum tomography technique for the quantum information acquisition to obtain the Rabi oscillation stabilization control law based on the root locus theory, which can be used to suppress the atomic spontaneous emission and the associated decoherence effect. Finally a physical implementation scheme of the strategy is given and the simulation results show that it can prevent the Rabi oscillation from vanishing and thus provide a stable environment for quantum computing.

2. Methods

2.1. The System Model. The cavity QED investigates the interaction of single atoms with single electromagnetic field modes, defined, for example, by a pair of mirrors illustrated in Figure 1 [6], which is a schematic representation of a cavity
QED system consisting of an atom with two energy levels interacting with a single photon mode trapped by mirrors to form a cavity. A photon in the cavity, bouncing back and forth between the mirrors, can be absorbed by the atom; conversely, if the atom is excited, it can decay by emitting a photon into the cavity. The rate of this atom-light interaction \( (g) \) is proportional both to the dipole moment of the atom and to the electric field of the photon at the atom's location.

The strong-coupling regime is reached when the interaction rate of the atom and a single photon \((g)\) is larger than the dissipation arising from the loss of photons (at rate \( \kappa \)) or from emission from the atom into other modes at rate \( \gamma \). The excited atoms will periodically release and absorb photons with a certain frequency, a phenomenon known as vacuum Rabi oscillations \([7]\). The presence of the cavity has made the spontaneous emission from the atom, known as vacuum Rabi oscillations \([7]\). The presence of the cavity has made the spontaneous emission from the atom, known as vacuum Rabi oscillations \([7]\).

Undesired processes can take place in any real system and the challenge for realizing strong-coupling cavity QED is that the generation of entanglement is to maximize the vacuum Rabi frequency while simultaneously to minimize the decoherence effects described by the decay \( (\kappa, \gamma) \). In this paper, the optical Bloch equations describing the mechanism of cavity QED are investigated to obtain the transfer function of the Rabi oscillation with the spontaneous emission \([8]\). A compensation strategy is designed to suppress the spontaneous emission of atoms, which has a negative effect on the coherence of the system. It should be noted that all of the following discussion is based on zero detuning as a preconditions.

Now we start from the optical Bloch equation of the cavity QED. The time-dependent mechanics of cavity QED is based on the time-dependent Schrödinger equation \([9]\):

\[
\hat{H}\psi(r, t) = \ii \hbar \frac{d\psi(r, t)}{dt}.
\]

We first investigate an isolated 2-level system \( |\psi_1\rangle, |\psi_2\rangle \) with energy eigenvalues \( E_1, E_2 \). The energy difference is related to the transition frequency \( 2\pi \omega_0 \), that is, \( \hbar \omega_0 = E_2 - E_1 \). Then we move forward to consider the effect on the atom of an incident light beam. Their interaction with the atom causes an additional electromagnetic energy \( H_I \) to the Hamiltonian of the system \( H_0 \). The total Hamiltonian is then \( H = H_0 + H_I \), which is explicitly dependent on time. In this case, specifying the vector of the light field \( E_0 \) pointing to the \( x \)-direction, if the frequency \( \omega \) of the light is close to \( \omega_0 \), only the two selected atomic states are involved in the radiative process. The solution to the Schrödinger equation (1) must be a linear superposition

\[
\psi(r, t) = C_1 \psi_1(r, t) + C_2 \psi_2(r, t)
\]

with \( \int dV|\psi(r, t)|^2 = |C_1|^2 + |C_2|^2 = 1 \).

Assume that the vector of the light field is \( E_0 \), and the total atomic electric dipole moment is \( J = -\varepsilon \sum r_j = -\varepsilon D \). The main contribution to the interaction Hamiltonian arises from the potential energy of this electric dipole in the electric field of the light beam. We can write

\[
H_I = eD \cdot E_0 \cos \omega t.
\]

Inserting (2) into (1), one obtains the equations for the coefficients \( C_1(t) \) and \( C_2(t) \):

\[
C_1 M_{11} + C_2 e^{-i\omega t} M_{12} = i \frac{dC_1}{dt},
\]

\[
C_1 e^{i\omega t} M_{21} + C_2 M_{22} = i \frac{dC_2}{dt},
\]

where \( M_{km} \) are the transition matrix elements: \( \hbar M_{km} = \int \psi_k^* \hat{H} \psi_m dV = \langle \psi_k | \hat{H} | \psi_m \rangle \). From symmetry one sees \( M_{11} = M_{22} = 0 \) and \( M_{12} = M_{21} = (1/\hbar) e \cdot E_0 X_{12} \cos(\omega t) \) where \( X_{12} = \int \psi_1^* X \psi_2 dV = \langle \psi_1 | \hat{X} | \psi_2 \rangle \) is the dipole matrix element.

Now, we define the Rabi frequency \( \Omega \) as

\[
\Omega = \frac{1}{\hbar} e \cdot E_0 X_{12}.
\]

Using these matrix elements, (4) can be now written as

\[
\Omega \cos \omega t e^{-i\omega t} C_2 = i \frac{dC_1}{dt},
\]

\[
\Omega^* \cos \omega t e^{i\omega t} C_1 = i \frac{dC_2}{dt}.
\]

For \( \omega_0 + \omega \gg \omega_0 - \omega \), we can neglect the fast oscillation terms \( (\omega + \omega_0)t \). The evolution will be governed by the slow oscillating terms. This approximation is called the Rotating Wave Approximation (RWA).

Using \( \cos \omega t = (e^{i\omega t} + e^{-i\omega t})/2 \), (6) can be rewritten as

\[
\Omega \frac{1}{2} e^{-i(\omega - \omega_0)t} C_2 = i \frac{dC_1}{dt},
\]

\[
\Omega^* e^{i(\omega - \omega_0)t} C_1 = i \frac{dC_2}{dt}.
\]

For zero detuning, \( \omega = \omega_0 \), one finds the well-known Rabi oscillations between the ground and excited states of the driven two-level system.

From the coefficients \( C_1(t) \) and \( C_2(t) \), we can form equations for the density matrix of the atom. Noticing the four elements of the atomic density matrix element \( \rho_{ij} \) defined...
by \( \rho_{11} = |C_1|^2, \rho_{12} = C_1 \overline{C}_2, \rho_{21} = C_1 \overline{C}_2 = \rho_{22} = |C_2|^2 \)
with the real diagonal elements satisfying \( \rho_{11} + \rho_{22} = 1 \) and the off diagonal elements satisfying \( \rho_{12} = \rho_{21} \), one can apply the RWA to find the equations of motion for the density matrix as follows:

\[
\frac{d\rho_{22}}{dt} = -i\frac{\rho_{11}}{2} - \frac{1}{2}i\Omega^* e^{i(\omega_0 - \omega)t} \rho_{12} + \frac{1}{2}i\Omega e^{-i(\omega_0 - \omega)t} \rho_{21},
\]

\[
\frac{d\rho_{12}}{dt} = -\frac{1}{2}i\Omega e^{-i(\omega_0 - \omega)t} (\rho_{11} - \rho_{22}).
\]

The previous discussions are concerned with the situation when there is no damping due to spontaneous emission. Now we consider the spontaneous emission; the rectified equations are as follows:

\[
\frac{d\rho_{22}}{dt} = -i\frac{\rho_{11}}{2} - \frac{1}{2}i\Omega^* e^{i(\omega_0 - \omega)t} \rho_{12} + \frac{1}{2}i\Omega e^{-i(\omega_0 - \omega)t} \rho_{21}
\]

\[-2\gamma \rho_{21},
\]

\[
\frac{d\rho_{12}}{dt} = -\frac{1}{2}i\Omega e^{-i(\omega_0 - \omega)t} (\rho_{11} - \rho_{22}) - \gamma \rho_{12},
\]

where \( \gamma \) is the atomic spontaneous emission damping ratio.

For the special initial conditions \( \rho = [1, 0, 0, 0]^T \) in the case of resonant light \( \omega = \omega_0 \), the optical Bloch equation degenerates into constant coefficient differential equations [9]:

\[
\frac{d\rho}{dt} = \begin{bmatrix}
0 & 2\gamma & \frac{1}{2}i\Omega^* & -\frac{1}{2}i\Omega \\
0 & -2\gamma & -\frac{1}{2}i\Omega^* & \frac{1}{2}i\Omega \\
-\frac{1}{2}i\Omega & \frac{1}{2}i\Omega & -\gamma & 0 \\
\frac{1}{2}i\Omega^* & -\frac{1}{2}i\Omega & 0 & -\gamma
\end{bmatrix} \rho
\]

\[
\rho(0) = [1 \ 0 \ 0 \ 0]^T.
\]

Noticing that \( \rho_{11} = \rho_{11}^*, \rho_{22} = \rho_{22}^* \), we can give a general solution of \( \rho_{22} \):

\[
\rho_{22} = \frac{|\Omega|^2}{4\gamma^2 + 2|\Omega|^2} \left[ 1 - \left( \cos \mu t + \frac{3\gamma}{2\mu} \sin \mu t \right) e^{-3\gamma t/2} \right]
\]

\[
\mu = \sqrt{|\Omega|^2 - \frac{1}{4}\gamma^2}.
\]

2.2. The Rabi Oscillation Stabilization. When external coherent laser field was applied, the vacuum-field-induced coherence effects will be replaced by the microwave-field-induced coherence effects. The decoherence effect caused by spontaneous emission in the system can be suppressed by the introduction of the control of the laser field. Furthermore, the method for implementing the decoherence suppression is to change the Rabi oscillation frequency. According to the previous strategy, the transfer function of the system is constructed and then the decoherence suppression is realized through the compensation of the transfer function.

We can infer from (11) that the underdamped Rabi oscillation is a typical second-order system and the open-loop transfer function is \( (0 < \xi < 1) \):

\[
G(s) = \frac{K_0 \omega_n^2}{s^2 + 2\xi \omega_n s + \omega_n^2}.
\]

Hence, the unit step response of the open-loop system described by (10) is as follows:

\[
y(t) = K_0 \left[ 1 - \left( \cos \omega_d t + \frac{\xi}{\sqrt{1 - \xi^2}} \sin \omega_d t \right) e^{-\xi \omega_d t} \right],
\]

where \( \omega_d = \sqrt{1 - \xi^2} \omega_n \).

Comparing formula (11) and (14), the parameters in the transfer function of damping Rabi oscillation can be obtained as follows:

\[
K_0 = \frac{|\Omega|^2}{4\gamma^2 + 2|\Omega|^2},
\]

\[
\xi = \frac{3\gamma}{\sqrt{4\mu^2 + 9\gamma^2}},
\]

\[
\omega_n = \frac{1}{2} \sqrt{4\mu^2 + 9\gamma^2}.
\]

If we put the open-loop transfer function (13) into a unit negative feedback system, the root locus of the closed-loop system is as Figure 2(a) shows. And the damping system is compensated on this basis. The basic idea is to make the unit step response of the compensated system become an equal amplitude oscillation through open-loop gain setting and pole-zero configuration. The problem is how to design the compensated system so that the root locus of the closed-loop system will pass through the imaginary axis, and at the same time, the operating point of the system is at the intersection of the root locus with the imaginary axis. A feasible solution to the problem is as follows.

(1) Add a pole \( s = -p \) in the negative half real axis, where \( p > \xi \omega_n \). After this step, the root locus of the system is as Figure 2(b) shows.

(2) Considering that the compensated system is sensitive to the open-loop gain after step (1), then we add a zero \( s = -\varepsilon \) to locate the asymptotes of the root locus in the right side of the imaginary axis. Let \( \Delta \chi > 0 \) be the intersection of the asymptotes and the real axis. To meet the requirements of the asymptote \((-p - 2\xi \omega_n + z)/2 = \Delta \chi\), we get \( z = p + 2\xi \omega_n + 2\Delta \chi \), where \( \Delta \chi \) should be moderately selected to avoid causing the open-loop gain to be too large. After this step, the root locus of the system is as Figure 2(c) shows.

According to the control theory, the closed-loop characteristic equation after the previous two steps is

\[
(s + p) \left( s^2 + 2\xi \omega_n^2 s + \omega_n^2 \right) + K_0 \omega_n^2 (s + z) = 0.
\]
The condition for a critical oscillation is that the poles of the closed-loop system are located on the imaginary axis. Letting $s = iy$ and inserting it into (17), we have

$$K = \frac{\xi}{\omega_n \Delta x} \left( p^2 + 2\xi\omega_n p + \omega_n^2 \right).$$  \hspace{1cm} (18)

Since $K_0$ has been considered as a part in the open-loop gain $K$, that is, $K = K' K_0$, we have

$$K' = \frac{\xi}{\omega_n \Delta x} \left( p^2 + 2\xi\omega_n p + \omega_n^2 \right) \left( \frac{4\gamma^2}{|\Omega|^2} + 2 \right).$$  \hspace{1cm} (19)

By inserting (12), (16) into (19), we get

$$K' = \frac{3\gamma \left( p^2 + 3\gamma\omega_n + 2\gamma^2 + |\Omega|^2 \right)}{\Delta x |\Omega|^2}.$$  \hspace{1cm} (20)

### 2.3. Physical Implementation

In the feedback control of the quantum system, the information of the density matrix cannot be measured directly because of the characteristics of the quantum system. One of the challenges exists in how to access the quantum information and feed it back to the input, in other words, how to construct the negative feedback channel for the quantum second-order system. In our work, for solving the problem of information acquisition of the quantum state, a quantum tomography scheme is designed to reconstruct the density matrix.

The physical implementation of the proposal is as Figure 3 shows. The detailed description of the steps is as follows: First, based on the tomography process, each element of the density matrix $\rho$ is reconstructed from the output; thus, the quantum information has been transformed into classical information and fed back to the input. In order to realize the compensation strategy of the Rabi oscillation based on the transfer function analysis, a compensation circuit is designed using the active phase-lead compensator and the double integral A/D converter. The quantum density matrix information is transformed into the classical voltage signal for driving the light beam, which can be used to stabilize the Rabi oscillation. The details are described in Sections 2.3.1 and 2.3.2.

#### 2.3.1. Information Acquisition

Quantum tomography technique is an indirect method to determine quantum system parameters. The basic idea is to construct multiple copies of the photon from the system output and determine density matrix elements of the output photon through the optical operations of the photon copies [10]. Assuming that the system output is single-qubit photon, the measurement strategy is as follows [11, 12].

1. Let the $N$ identical copies of the output photon pass through the horizontal-polarization wave plate, and record the number $n_0$.
2. Let the $N$ identical copies of the output photon pass through the vertically polarization wave plate and record the number $n_1$.
3. Let the $N$ identical copies of the output photon pass through the left-rotation wave plate and record the number $n_2$.
4. Let the $N$ identical copies of the output photon pass through the right-rotation wave plate and record the number $n_3$. 

![Figure 3: Schematic representation of the realization of the compensation network.](image-url)
The relationship between $n_i$ ($i = 0, 1, 2, 3$) and the system output $\rho_{\text{out}}$ can be described as follows [11,12]:

\begin{align}
    n_0 &= N \langle 0 | \rho_{\text{out}} | 0 \rangle, \\
    n_1 &= N \langle 1 | \rho_{\text{out}} | 1 \rangle, \\
    n_2 &= N \langle + | \rho_{\text{out}} | + \rangle, \\
    n_3 &= N \langle - | \rho_{\text{out}} | - \rangle. \\
\end{align}

(21)

The density matrix of output photon can be reconstructed according to $(n_0, n_1, n_2, n_3)$:

\begin{align}
    \rho_{\text{out}} &= \left[ \begin{array}{cccc}
        n_0 & n_1 & n_2 & n_3 \\
        n_0^* & n_0 + n_1 & n_2 & n_3^* \\
        n_1^* & n_0 + n_1 & n_2 + n_3 & -1/2 \\
        n_2^* & n_2 + n_3 & -1/2 & n_0 + n_1 \\
    \end{array} \right], \\
    \left( \begin{array}{c}
        n_2 \\
        n_0 + n_1 \\
        -1/2 \\
        n_0 + n_1 \\
    \end{array} \right)^T.
\end{align}

(22)

2.3.2. Compensation. If the element $\rho_{22}$ of the density matrix has been reconstructed by (21), a voltage signal proportional to $\rho_{22}$ can be obtained through the compensation to drive the light beam. The classical circuit to achieve this function consists of two parts.

(1) Due to the typical phase-lead compensation $D(s) = (s + z)/(s + p), (p > z)$, the implementation of the active phase-lead compensation network is as Figure 4 shows.

(2) Due to the $1/|\Omega|^2$ in the expression of $K'$, a double integral A/D converter can be used to realize the reciprocal operation of $|\Omega|^2$ as Figure 5 shows.

3. Results and Discussion

Through the previous analysis, a coherence preserving solution in cavity QED has been presented using the quantum tomography and the Rabi oscillation compensation. In the following, simulation results have been analyzed for the evaluation of the strategy.

3.1. Results of the Quantum Tomography. As stated in Section 2.3, we will let the copied output photons pass through four types of polarization wave plate and record the number of the photons passing through each type of the wave plate, respectively, for reconstructing the output density matrix. Taking into account the errors that may exist in the process, we should mention that there are mainly two kinds of errors in any realistic system: the first is the measurement error due to the accuracy and sensitivity of the experimental apparatus, the noise from the external environment, the random interference, and so forth; and the other one is the statistical error caused by the random collapse because of the measurement of the output state; that is, infinite times of detection are needed to obtain the accurate quantum information theoretically, which is impossible in practice.

In this simulation, a theoretical value of $n_i$ ($i = 0, 1, 2, 3$) can be calculated from (21). In order to investigate the error's effect on the reconstruction, a random interference is added on each value of $n_i$ ($i = 0, 1, 2, 3$) for calculating the output density matrix by (22). We can get the difference of each component of the density matrix between the target quantum state $\rho_{ij}$ and the reconstructed quantum state $\rho_{ij}'$ by

\[ \Delta \rho_{ij} = |\rho_{ij} - \rho_{ij}'|, \]

where the operator $|\cdot|$ stands for the magnitude of the error and as for the single-qubit quantum state, $i, j = 1, 2$.

In this paper, a series of error data are obtained by changing the number of the input photons. The relationship between the error and the number of the input photon is shown in Figure 6, from which the following conclusions can be drawn.

(1) Due to the presence of measurement error in the experiment, there is deviation between the statistical number of photons and the theoretical value, which will lead to the deviation between the reconstructed density matrix and the target quantum state density matrix. Therefore, the reconstructed density matrix may not satisfy the conditions of completely positive or preserving the trace, and this deviation is randomly generated and will have an inevitable impact on the results, which is more significant especially when the number of input photons is relatively small.
(2) According to the theory of quantum tomography, infinite times of detection are needed to guarantee a completely accurate reconstructed density matrix, which cannot be done in the experiment. However, as can be seen from the simulation results in Figure 6, with the number of photons increasing, the error would converge to a satisfactory extent; in particular, when the number of input photons reaches 3,000 or more, it is reasonable to say that the negative impact of the measurement errors and statistical errors is negligible.

(3) Though the error can be eliminated by infinitely increasing the number of input photons, doing so will significantly increase the cost and reduce the efficiency of the experiment. An appropriate number of input photons should be chosen to achieve a compromise between the error and efficiency.

3.2. Results of the Rabi Oscillation Stabilization. From the discussion in Section 2, in the atom light interactions, if there is no damping due to the spontaneous emission, the process is coherent and reversible. But if the decoherence caused by the spontaneous emission exists, in other words, $\gamma \neq 0$, the equal amplitude oscillation will change to a damped one, which will generate detrimental effects on quantum information processing. The impact of the decoherence caused by the spontaneous emission is as Figure 7 shows. At $t = 0$, the atom is in the ground state ($\rho_{11}(0) = 1, \rho_{22}(0) = 0$). The probability to find the atom in the excited state is plotted for various ratios of $\gamma$ and the Rabi frequency $\Omega$. In the simulation, we have chosen the following value: $\gamma = 0, \gamma = 0.1\Omega, \gamma = 0.25\Omega, \gamma = 0.5\Omega$, and $\gamma = \Omega$.

As can be seen from Figure 7, when $\gamma = 0$, the oscillation is with equal amplitude and fixed frequency. With the $\gamma$ increasing, the damping effect becomes more and more significant. The main objective of our design is to overcome the damping effect by compensation; that is to say, when $\gamma$ which stands for the spontaneous emission exists, the process will still be a coherent process with equal amplitude and fixed frequency.
According to the strategy described in Section 2, taking $\gamma = 0.3$, $|\Omega| = 2$, $p = 1.5$, and $\Delta x = 0.1$, the unit step response of the uncompensated and compensated system is shown in Figures 8(a) and 8(b), respectively.

It is clear that the uncompensated system approaches a constant value after the damping process and the compensated system can maintain a sustained oscillation with a constant frequency and amplitude, which have proved the effectiveness and superiority of our design.

4. Conclusions

For the coherence preservation in cavity QED, the model of the damping Rabi oscillation in the form of the transfer function is derived based on the optical Bloch equation. The transfer function of the damping Rabi oscillation is compensated using the root locus technique derived from the classical control theory to suppress the atom’s spontaneous emission. Finally, a physical implementation is put forward to keep the coherence in cavity QED. The strategy has provided a basis for the entanglement preparation in cavity QED theoretically. The research has theoretical significance and practical value. The simulation results showed that the compensated system can maintain a sustained oscillation with a constant frequency and amplitude. And it means the process is a coherent reversible one, which is an ideal environment for quantum information processing.

However, this work is based on the semiclassical optical Bloch equations. In other words, only the atom is quantized and the field is treated as a definite function of time rather than as an operator. To obtain more rigorous results, the further work will focus on the Jaynes-Cummings model, in
which the radiation field is also quantized. And meanwhile, an appropriate quantum feedback channel [13] is expected to be found to replace the current classical feedback channel.

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References

Review Article

A Survey of Quantum Lyapunov Control Methods

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The condition of a quantum Lyapunov-based control which can be well used in a closed quantum system is that the method can make the system convergent but not just stable. In the convergence study of the quantum Lyapunov control, two situations are classified: nondegenerate cases and degenerate cases. For these two situations, respectively, in this paper the target state is divided into four categories: the eigenstate, the mixed state which commutes with the internal Hamiltonian, the superposition state, and the mixed state which does not commute with the internal Hamiltonian. For these four categories, the quantum Lyapunov control methods for the closed quantum systems are summarized and analyzed. Particularly, the convergence of the control system to the different target states is reviewed, and how to make the convergence conditions be satisfied is summarized and analyzed.

1. Introduction

The theory of quantum mechanics is one of the major discoveries in the history of science in the 20th century. It is a very important issue to study the properties of the quantum mechanical systems and their control. According to whether the system is isolated or not, a quantum mechanical system can be a closed system or an open system. In a closed quantum system, the evolution of the state is unitary. There are mainly two methods to describe the evolution of a closed quantum system's states. They are the Schrödinger equation $i\dot{\psi}(t) = (H_0 + \sum_{k=1}^{r} H_k u_k(t))\psi(t)$ and the quantum Liouville equation $i\dot{\rho}(t) = [H_0 + \sum_{k=1}^{r} H_k u_k(t), \rho(t)]$, in which $|\psi(t)\rangle$ is the quantum state vector, $\rho(t)$ is the density operator, $H_0$ is the internal Hamiltonian, and $H_k, (k = 1, \ldots, r)$ are the control Hamiltonians. In an open quantum system, the system interacts with the surroundings, thus the loss of the system's information leads to the non-unitary evolution of the state. The most common method to describe the open system is the Lindblad master equation: $i\dot{\rho} = [H_0 + \sum_{k=1}^{r} H_k u_k(t), \rho] + L_D(\rho)$, which is in fact the sum of a closed system and a dissipative term caused by the loss of the information or energy. Obviously, the research of the properties of the closed quantum system and its control is relatively simple. Moreover, there is a more important fact: the research of the closed quantum system is the basis of that of the open quantum system.

Quantum control has attracted much attention in recent years and it has been found the potential applications in many fields such as atomic physics [1–4], molecular chemistry [5–9] and quantum information [10, 12]. Up to now, there have been many quantum methods, such as quantum optimal control [13–15], adiabatic control [16–18], the Lyapunov-based control [19–41], and optimal Lyapunov-based quantum control [42]. For the Lyapunov-based quantum control, it is relatively easy to design an analytical but not numerical control law, and the control system based on this control method is at least stable, so it has been a common control method.

One of the major concerns of the Lyapunov control is choosing an appropriate Lyapunov function to design the control laws. Ordinarily, the control laws and the control effects are different when the Lyapunov functions are distinct. It's a good idea to choose the Lyapunov function based on the geometrical and physical meanings. Usually, there are mainly three Lyapunov functions to be selected: the Lyapunov function based on the state distance [19–21, 26–32, 39–41], the state error [22, 23, 37, 38], and the average value of an imaginary mechanical quantity [24, 25, 39, 41]. The so-called imaginary mechanical quantity means that it is a linear Hermitian operator to be designed and may be not a physically meaningful observable quantity such as coordinate and energy. Among these three Lyapunov functions, the Lyapunov-based quantum control methods based on the state
distance and state error only need to adjust the scale factors of the control laws. These two Lyapunov control methods are relatively simple and easy to grasp. The Lyapunov-based quantum control based on the average value of an imaginary mechanical quantity contains more adjustable parameters. So it is more flexible and also more complex at the same time.

Generally speaking, the Lyapunov-based control method can only ensure that the control system is stable. The probability control in the quantum system requires us to design a control strategy which can make the system convergent, because a stable quantum control method may result in that the control system cannot reach the desired target state. Therefore another major concern of this control strategy for the closed quantum systems is the convergence of the control systems. So far, there have been the following research results on the convergence of the closed quantum systems [19, 23–25, 27–29, 33, 36].

(I) For the Schrödinger equation, the convergence conditions are as follows. (i) The internal Hamiltonian is strongly regular; (ii) All the eigenstates, which are different from the target state, are directly coupled to the target state for the Lyapunov control based on the state distance or the state error, or any two eigenstates are coupled directly for the Lyapunov control based on the average value of an imaginary mechanical quantity.

(II) For the quantum Liouville equation, the convergence conditions are as follows. (i) The internal Hamiltonian is strongly regular, and (ii) the control Hamiltonians are full connected.

At first, the Lyapunov control method which could only ensure the convergence to the target eigenstate was studied [19, 23, 25]. Then, the target mixed state, which commutes with the internal Hamiltonian, was studied [33, 36]. Later, the convergence to the target superposition state was solved by means of designing the control laws in the interaction picture of the control system, and the convergence to the target mixed state which does not commute with the internal Hamiltonian was solved by using a unitary transformation.

In fact, many actual systems do not satisfy the convergence conditions mentioned above, such as the time domain model of the selective excitation of the stimulated Raman scattering [43], the coupled two spin systems, and one-dimensional oscillators [44]. These systems are called non-ideal systems and in the degenerate cases. For the degenerate cases, the convergence of the control systems was solved by introducing a series of implicit function perturbations and choosing an implicit Lyapunov function [37–40]. At first, the convergence to the target eigenstate was only guaranteed [37–40]. Then the convergence to the target mixed state which commutes with the internal Hamiltonian was solved by introducing a series of implicit function perturbations, and the convergence to the target superposition state and the target mixed state which does not commute with the internal Hamiltonian was solved by introducing a series of constant disturbances.

The aim of this paper is to summarize and analyze the existing Lyapunov control methods for the nondegenerate and degenerate cases, respectively. Dividing the target state into four categories: the eigenstate, the mixed state which commutes with the internal Hamiltonian, the superposition state, and the mixed state which does not commute with the internal Hamiltonian state, we summarize the design methods of the control laws, analyze the convergence to the target state, and investigate how to make these conditions of the convergence be satisfied.

The remainder of this paper is arranged as follows. In Section 2, the research results for the nond-egenerate cases are summarized and analyzed. In Section 3, the research results for the degenerate cases are summarized and analyzed. Some concluding remarks are drawn in Section 4.

2. Non-Degenerate Cases

The design of the control laws and the analysis of the convergence are very important in the Lyapunov control method. The design of the control laws is based on the Lyapunov stability theorem, which is to design the control laws to make the selected positive semi-definite Lyapunov function $V(t)$ satisfy $V(t) \leq 0$. The convergence analysis of this control method is mainly based on the LaSalle invariance principle [44] for the autonomous systems, or the improved Barbalat lemma [45] for the non-autonomous systems.

In this Section, we will summarize and analyze the research results on the convergence of the control system in the non-degenerate cases for the target state being an eigenstate, a mixed state which commutes with the internal Hamiltonian, the superposition state, or/and a mixed state which does not commute with the internal Hamiltonian state, respectively.

2.1. Target Eigenstate. It is convenient to use the bilinear Schrödinger equation to describe the control systems if the target state is a pure state. Consider the $N$-level closed quantum system governed by the following bilinear Schrödinger equation:

$$i |\psi(t)\rangle = \left( H_0 + \sum_{k=1}^{r} H_k u_k(t) \right) |\psi(t)\rangle,$$

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

In the following sections, in the case that the target state $|\psi_f\rangle$ is an eigenstate, that is, $H_0|\psi_f\rangle = \lambda_f|\psi_f\rangle$, where $\lambda_f$ is the eigenvalue of the internal Hamiltonian $H_0$, the research results on the convergence are summarized and analyzed for the Lyapunov control based on the state distance, the state error, and the average value of an imaginary mechanical quantity, respectively.

2.1.1. Lyapunov Control Based on State Distance. Consider the following Lyapunov function based on the state distance:

$$V_1 (|\psi\rangle) = \frac{1}{2} \left( 1 - |\langle \psi | \psi_f \rangle|^2 \right).$$

The scientific world journal (II) For the quantum Liouville equation, the convergence conditions are as follows. (i) The internal Hamiltonian, $H_0$, is strongly regular; (ii) All the eigenstates, which are different from the target state, are directly coupled to the target state for the Lyapunov control based on the state distance or the state error, or any two eigenstates are coupled directly for the Lyapunov control based on the average value of an imaginary mechanical quantity.

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The design of the control laws and the analysis of the convergence are very important in the Lyapunov control method. The design of the control laws is based on the Lyapunov stability theorem, which is to design the control laws to make the selected positive semi-definite Lyapunov function $V(t)$ satisfy $V(t) \leq 0$. The convergence analysis of this control method is mainly based on the LaSalle invariance principle [44] for the autonomous systems, or the improved Barbalat lemma [45] for the non-autonomous systems.

In this Section, we will summarize and analyze the research results on the convergence of the control system in the non-degenerate cases for the target state being an eigenstate, a mixed state which commutes with the internal Hamiltonian, the superposition state, or/and a mixed state which does not commute with the internal Hamiltonian state, respectively.

2.1. Target Eigenstate. It is convenient to use the bilinear Schrödinger equation to describe the control systems if the target state is a pure state. Consider the $N$-level closed quantum system governed by the following bilinear Schrödinger equation:

$$i |\psi(t)\rangle = \left( H_0 + \sum_{k=1}^{r} H_k u_k(t) \right) |\psi(t)\rangle,$$

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

In the following sections, in the case that the target state $|\psi_f\rangle$ is an eigenstate, that is, $H_0|\psi_f\rangle = \lambda_f|\psi_f\rangle$, where $\lambda_f$ is the eigenvalue of the internal Hamiltonian $H_0$, the research results on the convergence are summarized and analyzed for the Lyapunov control based on the state distance, the state error, and the average value of an imaginary mechanical quantity, respectively.

2.1.1. Lyapunov Control Based on State Distance. Consider the following Lyapunov function based on the state distance:

$$V_1 (|\psi\rangle) = \frac{1}{2} \left( 1 - |\langle \psi | \psi_f \rangle|^2 \right).$$

The aim of this paper is to summarize and analyze the existing Lyapunov control methods for the nondegenerate and degenerate cases, respectively. Dividing the target state into four categories: the eigenstate, the mixed state which commutes with the internal Hamiltonian, the superposition state, and the mixed state which does not commute with the internal Hamiltonian state, we summarize the design methods of the control laws, analyze the convergence to the target state, and investigate how to make these conditions of the convergence be satisfied.

The remainder of this paper is arranged as follows. In Section 2, the research results for the nond-egenerate cases are summarized and analyzed. In Section 3, the research results for the degenerate cases are summarized and analyzed. Some concluding remarks are drawn in Section 4.
The time derivative of the Lyapunov function (2) is
\[
\dot{V}_1 = - \sum_{k=1}^{r} u_k(t) \cdot \text{Im} \left[ \langle \psi | \psi_f \rangle \langle \psi_f | H_k | \psi \rangle \right].
\]
(3)

The control laws \( u_k(t) \) which can make \( \dot{V}_1 \leq 0 \) hold can be designed as
\[
u_k(t) = K_k f_k \left( \text{Im} \left[ \langle \psi | \psi_f \rangle \langle \psi_f | H_k | \psi \rangle \right] \right),
\]
\[
(k = 1, \ldots, r),
\]
(4)

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

The control laws designed in (4) can only ensure the control system governed by (1) to be stable. One needs to do further study on the convergence of the control system. The control system governed by (1) is an autonomous system, whose convergence can be analyzed based on the LaSalle invariance principle [44]. According to the LaSalle invariance principle, as \( t \to \infty \), any state trajectory will converge to the largest invariant set contained in the set \( E \) in which the states satisfy that the first order derivative of the Lyapunov function equals zero. In fact, the set \( E \) contains not only the target state but also other states, thus the system may converge to other states rather than the target state. The main idea to solve this problem is to add restrictions to make the set \( E \) as small as possible. Based on the LaSalle invariance principle, the convergence of the control system governed by (1) can be depicted by Theorem 1.

**Theorem 1** (see [19]). Consider the control system governed by (1) with control fields \( u_k(t) \) designed in (4). If (i) the system is strongly regular, that is, \( \omega_{ij} \neq \omega_{lm}, (i', j') \neq (l, m), i', j', l, m \in \{1, 2, \ldots, N\}, \omega_{lm} = \lambda_l - \lambda_m, \) where \( \lambda_l \) is the \( l \)-th eigenvalue of \( H_0 \) corresponding to the eigenstate \( \langle \phi_l | \) (ii) for any \( \langle \phi_{ij} | \neq | \psi_f \rangle, i \in \{1, 2, \ldots, N\}, \) there exists at least a \( k \in \{1, \ldots, r\} \) such that \( \langle \phi_l | H_k | \psi_f \rangle \neq 0, \) then any state trajectory will converge toward \( E_1 = \{e^{i\theta} | \psi_f \rangle, \theta \in \mathbb{R} \}. \)

From Theorem 1, one can see that in the case that the target state is an eigenstate, if the control system governed by (1) satisfies the conditions (i)-(ii), the control system can converge to the equivalent state of the target eigenstate \( e^{i\theta} | \psi_f \rangle \) from any initial pure state. These two conditions are relevant to the internal Hamiltonian and the control Hamiltonians, which are system parameters. Once the control system is determined, the Hamiltonians are fixed and cannot be changed by designing the control laws.

**2.1.2. Lyapunov Control Based on State Error.** Consider the following Lyapunov function based on the state error:
\[
V_2(\langle \psi |) = \frac{1}{2} \langle \psi - \psi_f | \psi - \psi_f \rangle.
\]
(5)

In the case of selecting the Lyapunov function based on the state error defined by (5), in order to facilitate to design the control laws based on the Lyapunov stability theorem, the drift item appeared in the first order time derivative of Lyapunov function, which is caused by the internal Hamiltonian, is needed to be eliminated. The existing solution is to add a global phase control item \( \omega \) into the control system governed by (1). This method will not change the population distribution of the control system. Thus the dynamical equation (1) becomes
\[
\dot{\psi}(t) = \left( H_0 + \sum_{k=1}^{r} H_k u_k(t) + \omega I \right) | \psi(t) \rangle.
\]
(6)

After some deduction, one can obtain the time derivative of the Lyapunov function (5) as
\[
\dot{V}_2 = - \left( \lambda_f + c \right) \mathfrak{F} \left( \langle \psi_f | \psi \rangle \right) - \sum_{k=1}^{r} \mathfrak{F} \left( \langle \psi_f | H_k | \psi \rangle \right) u_k(t).
\]
(7)

The control laws which can make \( \dot{V}_2 \leq 0 \) hold can be designed as
\[
\omega = - \lambda_f + cf_0 \left( \mathfrak{F} \left( \langle \psi_f | \psi \rangle \right) \right),
\]
(8)
\[
u_k(t) = K_k f_k \left( \mathfrak{F} \left( \langle \psi_f | H_k \rangle \psi \rangle \right) \right),
\]
(9)

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

Based on the LaSalle invariance principle, the convergence of the control system governed by (6) can be depicted by Theorem 2.

**Theorem 2** (see [19, 23]). Consider the control system governed by (6) with control fields \( u_k(t) \) designed in (9) and \( \omega \) designed in (8). If (i) \( \omega_{ij} \neq \omega_{lm}, (i', j') \neq (l, m), i', j', l, m \in \{1, 2, \ldots, N\}, \omega_{lm} = \lambda_l - \lambda_m, \) where \( \lambda_l \) is the \( l \)-th eigenvalue of \( H_0 \) corresponding to the eigenstate \( \langle \phi_l | \), (ii) for any \( \langle \phi_{ij} | \neq | \psi_f \rangle, i \in \{1, 2, \ldots, N\}, \) there exists at least a \( k \in \{1, \ldots, r\} \) such that \( \langle \phi_l | H_k | \psi_f \rangle \neq 0. \) Then any state trajectory will converge toward \( E_2 = \{e^{i\theta} | \psi_f \rangle, \theta \in \mathbb{R} \}. \)

From Theorem 2, one can see that for the case that the target state is an eigenstate, if the control system governed by (6) satisfies the conditions (i)-(ii), the control system can also converge to the equivalent state of the target eigenstate \( e^{i\theta} | \psi_f \rangle \) from any initial pure state.

**2.1.3. Lyapunov Control Based on Average Value of an Imaginary Mechanical Quantity.** Consider the following Lyapunov function based on the average value of an imaginary mechanical quantity:
\[
V_3(\langle \psi |) = \left( \langle \psi | P | \psi \rangle \right),
\]
(10)

where the imaginary mechanical quantity \( P \) is a positive definite Hermitian operator.

The first order time derivative of the Lyapunov function (10) can be obtained as
\[
\dot{V}_3 = i \langle \psi | [H_0, P] | \psi \rangle + i \sum_{k=1}^{r} \langle \psi | [H_k, P] | \psi \rangle u_k(t).
\]
(11)
Set \([H_0, P] = 0\) such that the drift term in the right side of (11) can be eliminated. In order to ensure \(V_3 \leq 0\), one can design \(u_k(t)\) as

\[
u_k(t) = -K_k f_k \left( i \langle \psi | [H_k, P] | \psi \rangle \right), \quad (k = 1, \ldots, r), \tag{12}
\]

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

Then based on the LaSalle invariance principle, all the state trajectories of the system will converge to the invariant set contained in the set \(E\) in which \(V = 0\) holds. Denote the state at the time \(t\) as \(|\psi(t)\rangle = \sum_{j=1}^{N} c_j(t) |\phi_j\rangle\), where \(c_j(t)\) is the coefficient corresponding to the \(j\)th eigenstate \(|\phi_j\rangle\).

For the Schrödinger equation governed by (1), if the control system is strongly regular and any eigenstate is directly coupled to all other eigenstates, that is, for any \(j \neq l, l, j \in \{1, 2, \ldots, N\}\), there exists a \(k \in \{1, \ldots, r\}\) such that \(\langle \phi_l | H_k | \phi_l \rangle \neq 0\), then one can deduce that \(V_3(t) = 0\) holds for all \(t \geq t_0, t_0 \in R\) is equivalent to

\[
(P_l - P_j) c_j (t_0) c_l^* (t_0) = 0, \quad (l, j = 1, \ldots, N), \tag{13}
\]

where \(P_l\) and \(P_j\) are the \(l\)th and \(j\)th eigenvalues of \(P\), respectively.

If the target state \(|\psi_f\rangle\) is an eigenstate, and all the eigenvalues of \(P\) are designed mutually different, that is, \(P_l \neq P_j\) for any \(l \neq j, (l, j = 1, 2, \ldots, N)\), then (13) is equivalent to

\[
c_j c_l^* = 0, \quad (l, j = 1, \ldots, N). \tag{14}
\]

Equation (14) implies that there is at most one \(c_j \neq 0, (j = 1, \ldots, N)\): that is, the system will converge to an eigenstate with \(t \to \infty\). Thus the convergence of the control system (1) can be depicted by Theorem 3.

**Theorem 3** (see [19, 24, 25]). Consider the control system governed by (1) with the control fields \(u_k(t)\) designed in (12). If (i) \(\omega_{l,j}^2 = \omega_{m,n} (l', m') \neq (l, m), l', m' \in \{1, \ldots, N\}, 
\omega_m = \lambda_m - \lambda_n\) where \(\lambda_i\) is the \(i\)th eigenvalue of \(H_0\) corresponding to the eigenstate \(|\phi_i\rangle\); (ii) for any \(l \neq j, i, j \in \{1, \ldots, N\}\), there exists at least one \(k \in \{1, \ldots, r\}\) such that \(\langle \phi_l | H_k | \phi_j \rangle \neq 0\); (iii) \([H_0, P] = 0\); (iv) for any \(l \neq m \in \{1, 2, \ldots, N\}\), \(P_l \neq P_m\) holds, where \(P_l\) is the \(l\)th eigenvalue of \(P\).

Then any state trajectory will converge toward \(E_3 = e^{i\theta} |\phi_i\rangle, i \in \{1, \ldots, N\}, \theta \in R\).

From Theorem 3, one can see that the control system will converge from any initial pure state to an eigenstate which may not be the target eigenstate. In order to make the system converge to the target eigenstate \(|\psi_f\rangle\) from any initial pure state \(|\psi_0\rangle\), as \(V_3(t) \leq 0\), one can add a restriction as

\[
V_3(|\psi_f\rangle) < V_3(|\psi_0\rangle) < V_3(|\psi_{other}\rangle), \tag{15}
\]

where \(|\psi_0\rangle\) is the initial state, \(|\psi_{other}\rangle\) represents any other state in the set \(E_3\) except the target state.

In such a way, any state trajectory of the system will converge to \(e^{i\theta} |\psi_f\rangle\) from any initial pure state \(|\psi_0\rangle\).

Next, let us analyze how to make these convergence conditions be satisfied. Conditions (i) and (ii) are only relevant to the internal Hamiltonian \(H_0\) and the control Hamiltonians \(H_k, (k = 1, \ldots, r)\) which cannot be changed by designing appropriate control laws. Condition (iii) means that \(P\) and \(H_0\) have the same eigenstates. In order to make condition (iii) be satisfied, the eigenvalues of \(P\) can be designed as

\[
P = \sum_{j=1}^{N} P_j |\phi_j\rangle \langle \phi_j|.
\]

Because \(P\) should be positive definite, one needs to design \(P_l > 0, (i = 1, \ldots, N)\). The restriction (15) can be satisfied by means of designing an appropriate \(P\). For the restriction (15), Grivopoulos and Bamieh proposed a design principle of \(P\) to make \(V_3(|\psi_f\rangle) < V_3(|\psi_{other}\rangle)\) hold. This design principle of \(P\) can be depicted by Proposition 4.

**Proposition 4** (see [25]). With the constraint condition \(|\psi | \psi \rangle = 1\), the set of critical points of the Lyapunov function \(V_3(|\psi\rangle) = \langle \psi | P | \psi \rangle\) is given by the normalized eigenvectors of \(P\). The eigenvectors with the largest eigenvalue are the maxima of \(V_3\), the eigenvectors with the smallest eigenvalue are the minima and all others are saddle points.

According to Proposition 4, in order to make \(V_3(|\psi_f\rangle) < V_3(|\psi_{other}\rangle)\), \(P_l > P_j, (i = 1, \ldots, N, P_l \neq P_j)\) needs to be designed, where \(P_l\) is the eigenvalue of \(P\) corresponding to \(|\psi_l\rangle\). Then let us consider the whole restriction (15); it is an attraction problem. If the eigenvalues of \(P\) except \(P_l\) are close together, the attraction region will be very large. For the limiting case \(P_l = P_j > P_i > 0, (i \neq j, P_l, P_j \neq P_i)\), the attraction region will be the whole state space. Thus the design principle of \(P\) is \(P_l > P_j, (i = 1, \ldots, N, P_l \neq P_j)\) and to make \(P_l, P_l \neq P_j\) close together.

In conclusion, for the target state being an eigenstate, the design principle of \(P\) is as follows:

(i) \(P_l > P_m > 0\) for any \(l \neq m \in \{1, 2, \ldots, N\},\)

(ii) \(P_l > P_j, (i = 1, \ldots, N, P_l \neq P_j)\), \(P_l, P_l \neq P_j\) are close together,

(iii) Equation (16): \(P = \sum_{j=1}^{N} P_j |\phi_j\rangle \langle \phi_j|\).

From the above analyses, we can conclude that the Lyapunov control method based on the imaginary mechanical quantity proposed in [19, 24, 25] can only ensure the convergence to an eigenstate, but cannot guarantee the convergence to the target eigenstate from any initial pure state. However, if there exists a \(P\) to make the restriction (15) hold, then any state trajectory of the system will converge to the equivalent state of the target eigenstate \(e^{i\theta} |\psi_f\rangle\) from any initial pure state.
2.1.4. Relations between Three Lyapunov Functions. In the Liouville space, the Hilbert-Schmidt distance between two density operators $\rho_1$ and $\rho_2$ is

$$d_{\text{HS}}(\rho_1, \rho_2) = \sqrt{\text{tr}((\rho_1 - \rho_2)^2)}.$$  \hspace{1cm} (17)

The inner product of two operators $A$ and $B$ is defined as $\langle A | B \rangle = \text{tr}(A^\dagger B)$, where the operation $A^\dagger$ refers to the conjugate transpose of $A$. Because $\rho = |\psi\rangle \langle \psi|$, the square of the Hilbert-Schmidt distance between the density operator $\rho$ and the target density operator $\rho_f$ can be deduced as

$$d_{\text{HS}}^2(\rho, \rho_f) = 2 \left(1 - \left|\langle \psi | \psi_f\rangle\right|^2\right). \hspace{1cm} (18)$$

One can conclude from (18) that the Lyapunov function based on the state distance $V_1(|\psi\rangle) = (1/2)(1 - |\langle \psi | \psi_f\rangle|^2)$ and the state error $V_2(|\psi\rangle) = (1/2)(|\psi - \psi_f| - |\psi - \psi_f|)$ are equivalent.

For the Lyapunov function based on the average value of an imaginary mechanical quantity $V_3(|\psi\rangle) = |\psi|P|\psi\rangle$, if the imaginary mechanical quantity $P = (1/2)(I - |\psi_f\rangle\langle \psi_f|)$, $V_3(|\psi\rangle)$ will become $V_1(|\psi\rangle)$ [19]. Therefore $V_1(|\psi\rangle)$ is formally a special case of $V_3(|\psi\rangle)$.

In fact, $V_1(|\psi\rangle), V_2(|\psi\rangle),$ and $V_3(|\psi\rangle)$ can be unified in the following quadratic Lyapunov function:

$$V_4(|\psi\rangle) = \left\langle \psi - \alpha \psi_f \right| Q \left| \psi - \alpha \psi_f \right\rangle$$ \hspace{1cm} (19)

Next, we consider three cases as follows:

(i) $\alpha = 0, Q = (1/2)(I - |\psi_f\rangle\langle \psi_f|), V_4(|\psi\rangle)$ will reduce to $V_1(|\psi\rangle)$;

(ii) $\alpha = 1, Q = (1/2)I, V_4(|\psi\rangle)$ will reduce to $V_2(|\psi\rangle)$;

(iii) $\alpha = 0, V_4(|\psi\rangle)$ will reduce to $V_3(|\psi\rangle)$.

We can see that $V_1(|\psi\rangle), V_2(|\psi\rangle),$ and $V_3(|\psi\rangle)$ are special cases of $V_4(|\psi\rangle)$.

From the above analyses, we can conclude that all these three Lyapunov control methods can converge to the equivalent state of the target eigen state from any initial pure state. The Lyapunov control methods based on the state distance and the state error have only one adjustable parameter. So these two methods are very easy to grasp and very simple. The Lyapunov control based on the average value of an imaginary mechanical quantity has more adjustable parameters. So it is more flexible and also more complex at the same time. For the target eigenstate, $V_1(|\psi\rangle)$ and $V_2(|\psi\rangle)$ are equivalent, so the Lyapunov control based on the state distance and the state error have similar control effects. Because $V_1(|\psi\rangle)$ is formally a special case of $V_3(|\psi\rangle)$, generally, the control effect of the Lyapunov control based on the average value of an imaginary mechanical quantity is better than that of the state distance. At least, it can get the same control effect as the Lyapunov control of the state distance.

2.2. Target Mixed State Which Commutes with the Internal Hamiltonian. The bilinear Schrödinger equation cannot describe the mixed state. Thus for the target mixed state, it needs to use the quantum Liouville equation which can describe the evolution of any state of a closed quantum system. Consider the $N$-level closed quantum system governed by the following quantum Liouville equation:

$$i\dot{\rho}(t) = H_0 + \sum_{k=1}^{r} H_k u_k(t), \rho(t), \hspace{1cm} (20)$$

where $\rho(t)$ is the density operator.

Consider the Lyapunov function based on the average value of an imaginary mechanical quantity:

$$V_5(\rho) = \text{tr}(P\rho). \hspace{1cm} (21)$$

By means of setting $[H_0, P] = 0$, the first order time derivative of the Lyapunov function (21) can be deduced as

$$\dot{V}_5 = -i \text{tr}([P, H_0]\rho) - i \sum_{k=1}^{r} \text{tr}([P, H_k]\rho) u_k. \hspace{1cm} (22)$$

In order to ensure $\dot{V}_5 \leq 0$, one can design $u_k(t)$ as

$$u_k(t) = i\varepsilon_k \text{tr}([P, H_k]\rho), \hspace{1cm} (k = 1, \ldots, r), \hspace{1cm} (23)$$

where $\varepsilon_k \in R, \varepsilon_k > 0$.

Next, let us analyze the convergence to the target state. For the control system governed by (20) in the non-degenerate case, one can deduce that $V_5(t) = 0$ holds for all $t \geq t_0$, $t_0 \in R$ is equivalent to

$$(H_k)_{ij} (P_l - P_j) \rho_{lj} = 0, \hspace{1cm} j, l = 1, \ldots, N, \hspace{1cm} j < l, \hspace{1cm} (24)$$

where $\rho_{lj}(t)$ is the $(l, j)$th element of the state $\rho(t)$. If the target state $\rho_f$ commutes with $H_0$, that is, $[H_0, \rho_f] = 0$, and all the eigenvalues of $P$ are designed mutually different, that is, $P_l \neq P_j$ for any $l \neq j, l = 1, 2, \ldots, N$, then (24) is equivalent to

$$\rho_{lj} = 0, \hspace{1cm} (l, j = 1, \ldots, N) \hspace{1cm} (25)$$

which implies that the system will converge to a state which commutes with $H_0$. Thus based on the LaSalle invariance principle, the convergence of the control system governed by (20) can be depicted by Theorem 5.

**Theorem 5 (see [37])**. Consider the control system governed by (20) with the control field $u_k(t)$ designed in (23). If (i) the internal Hamiltonian is strongly regular, that is, $\omega_{i,j} \neq \omega_{m,n}, (i', j') \neq (l, m), i', j', l, m \in \{1, \ldots, N\}, \omega_{lm} = \lambda_i - \lambda_m$, where $\lambda_i$ is the $i$th eigenvalue of $H_0$ corresponding to the eigenstate $|\phi_i\rangle$; (ii) the control Hamiltonians are full coupled; that is, $\forall j \neq l$, for $k = 1, \ldots, r$, there exists at least a $(H_k)_{jl} \neq 0$; (iii) $[H_0, P] = 0$; (iv) $P_l \neq P_m, l \neq m \in \{1, 2, \ldots, N\}$, where $P_l$ is the $l$th eigenvalue of $P$. Then any state trajectory will converge toward $E_k = \{|\rho| \text{ tr}(\rho)| = 0, i, j \in \{1, 2, \ldots, N\} \}$, where $|\rho|_{ij}$ is the $(l, i)$th element of $\rho$.

From Theorem 5, one can see that if the control system satisfies the conditions (i)-(iv), the control system will converge from any initial state to a state that commutes with the
internal Hamiltonian, which may not be the target state. Next, what we need to do is to make the control system converge to the target state.

Denote the state in $E_4$ as $\rho_{E_4}$; then $[\rho_{E_4}, H_0] = 0$ holds which implies that $\rho_{E_4}$ and $H_0$ have the same eigenstates. Since the evolution of $\rho(t)$ is unitary, $\rho(t)$ for $t \geq 0$ are isospectral. So the eigenvalues of $\rho_{E_4}$ are a permutation of the eigenvalues of $\rho_0$. Thus the set $E_4$ has countable elements. If the initial state is generic, that is, the eigenvalues of the initial state are mutually different, the set $E_4$ will have $N!$ elements. For the target state $\rho_f$ which commutes with the internal Hamiltonian, that is, $[\rho_f, H_0] = 0$, in order to make the system converge to the target state $\rho_f$ which commutes with $H_0$ from any initial state $\rho_0$, Kuang and Cong proposed a restriction as

$$V_5(\rho_f) < V_5(\rho_0) < V_5(\rho_{\text{other}}),$$

(26)

where $\rho_{\text{other}}$ represents any other state in the set $E_4$ except the target state $\rho_f$.

In such a way, if there exists a $P$ to make the restriction (26) hold, any state trajectory of the system will converge to the target state $\rho_f$ which commutes with $H_0$ from any initial state $\rho_0$.

For how to make conditions (iii)-(iv) to be satisfied, please see Section 2.1.3. One can deduce the design principle of $P$ such that $V_5(\rho_f) < V_5(\rho_{\text{other}})$, the result can be depicted by Proposition 6.

**Proposition 6.** If $(\rho_f)_{ii} < (\rho_f)_{jj}$, $1 \leq i, j \leq N$, then one can design $P_1 > P_j$; if $(\rho_f)_{ii} = (\rho_f)_{jj}$, $1 \leq i, j \leq N$, then one can design $P_1 \neq P_j$; else if $(\rho_f)_{ii} > (\rho_f)_{jj}$, $1 \leq i, j \leq N$, then one can design $P_1 < P_j$, thus $V_5(\rho_f) < V_5(\rho_{\text{other}})$ holds, where $(\rho_f)_{ii}$ is the $(i,i)$th element of $\rho_f$.

It is difficult to design $P$ such that (26) holds for any initial state $\rho_0$ and any target state $\rho_f$ which satisfies $[\rho_f, H_0] = 0$. One possible method is to introduce a series of implicit function perturbations into the control laws, this method will be presented in Section 3.3.

For the target state $\rho_f$ which commutes with the internal Hamiltonian, the design principle of $P$ is as follows:

(i) $P_1 > P_m > 0$ for any $l \neq m \in \{1, 2, \ldots, N\}$;
(ii) Design $P$ according to Proposition 6;
(iii) Equation (16): $P = \sum_{i=1}^{N} P_{ij} |\phi_i\rangle \langle \phi_i|.$

In conclusion, if the control system satisfies the conditions (i)-(iv) in Theorem 5 and there exists a $P$ to make the restriction (26) hold, any state trajectory of the system will converge to the target mixed state $\rho_f$, which commutes with the internal Hamiltonian from any initial state $\rho_0$.

2.3. Target Superposition State. From Section 2.1.3, one can see that for the control system governed by (1), $\dot{V}(t) = 0$ holds for all $t \geq t_0, t_0 \in R$ is equivalent to $(\bar{P} - P)\rho \dot{c}_f^* = 0, (l, j = 1, \ldots, N)$. If the target state is a superposition state as $|\psi_f\rangle = \sum_{d=k_1}^{k_0} c_d |\phi_d\rangle, (1 \leq k_1 < k_0 \leq N)$, one can design $P_{k_1} = P_{k_2} = \cdots = P_{k_0}$ and other eigenvalues of $P$ are mutually different, then $(\bar{P} - P)\rho \dot{c}_f^* = 0, (l, j = 1, \ldots, N)$ is equivalent to

$$c_i \dot{c}_j^* = 0, \quad (l, j = 1, \ldots, N, l \neq k_1, \ldots, k_0).$$

(27)

Equation (27) implies that the system will converge to the set $E_5 = \text{span}(|\phi_{k_1}\rangle, |\phi_{k_2}\rangle, \ldots, |\phi_{k_0}\rangle)$, which means that the set $E_5$ contains infinite elements. Therefore this control method cannot ensure the system converge to the target superposition state by adding the restriction defined by (15). But this control method can ensure that the system will converge to the superposition of the eigenstates corresponding to target state. In fact, once one element of $P$ changes, all the populations of the levels will change accordingly. Therefore when there are not very many eigenstates corresponding to target state, the system maybe converge to the target state by regulating the eigenvalues of $P$. Otherwise, the system maybe cannot converge to the target state. Consider the extreme situation in which the target state is the superposition of all the eigenstates. According to the design principle of $P$, we should design $P = c_i I$, where $c_i$ is a real number, and $I$ is the unit matrix. Obviously, in this special case, the control method proposed in Section 2.1.3 will become invalid.

From Section 2.2, one can see that, for the control system governed by (20), $\dot{V}(t) = 0$ holds for all $t \geq t_0, t_0 \in R$ is equivalent to $(H_0)_{ij} (P_1 - P_2) (\rho(t)) = 0, j, l = 1, \ldots, N, j < l$. Consider the target state which does not commute with $H_0$, which includes the superposition state and the mixed state which does not commute with $H_0$. Without loss of generality, assume $(\rho_f)_{NN} \neq 0$; one can design $P_1 = P_2 = P_m$, thus the system will converge to $E_6 = \{\rho|\rho_1\} = 0, (l, j) \neq (3, N), (l, j) \neq (N, 3), j, l \in \{1, \ldots, N\}$. Because the set $E_6$ has infinite elements, this control method also cannot ensure the system will converge to the target state by adding the restriction defined by (26). But when the target state does not have so many nonzero off-diagonal elements, the system maybe converges to the target state by regulating the diagonal elements of $P$. When there are many nonzero off-diagonal elements in the target state, the degree of freedom of $P$ may be not enough.

From the above analyses, we can conclude that by means of using the control methods proposed in Sections 2.1 and 2.2, the control system may but cannot be ensured to converge to the target superposition state. This problem can be solved by means of designing the control laws in the interaction picture of the control system.

Consider the $N$-level control system in the interaction picture as

$$i \frac{\partial}{\partial t} \rho(t) = \sum_{k=1}^{r} H_k(t) u_k(t), \quad (\rho(t)).$$

(28)

Choose the Lyapunov function based on the average value of an imaginary mechanical quantity defined by (21). The first order time derivative of the Lyapunov function (21) can be obtained as

$$\dot{V}_5 = - \sum_{k=1}^{r} u_k(t) tr (i H_k(t) [\rho(t), P]).$$

(29)
To ensure $V_S \leq 0$, one can design $u_k(t)$ as

$$u_k(t) = -K_k \text{tr}(ih_k(t) \langle \rho(t), P \rangle), \quad K_k > 0, \quad (30)$$

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

The control system governed by (28) is a non-autonomous system; thus the LaSalle invariance principle cannot be used to analyze the convergence. One can use the improved Barbalat lemma which can be used for the non-autonomous system. According to the improved Barbalat lemma, the convergence of the control system governed by (28) can be depicted by Theorem 7.

**Theorem 7.** Consider the control system governed by (28) with the control field $u_k(t)$ designed in (30). If (i) the internal Hamiltonian is strongly regular; (ii) the control Hamiltonians are full connected, then any state trajectory will converge to the limit set $\mathcal{R}_1 \equiv \{ \rho_1 : [\rho_1, P] = 0 \}$ at $t \to \infty$, where $D$ is a diagonal matrix.

For the case that $P$ is chosen as a diagonal matrix, the limit set is reduced to $\mathcal{R}_1 = \{ \rho_1 : [\rho_1, P] = 0 \}$. For the case that $P$ is chosen as a nondiagonal matrix, if rank $\bar{A}(\bar{P}) = n^2 - n$ holds, then the limit set $\mathcal{R}_1$ is regular; namely, $\mathcal{R}_1 \equiv \{ \rho_1 : [\rho_1, P] = 0 \}$, where $\bar{A}(\bar{P})$ is the first $n^2 - n$ rows of $A(\bar{P})$, $A(\bar{P})$ is the real $(n^2 - 1) \times (n^2 - 1)$ matrix corresponding to the Bloch representation of $Ad_P$, and $Ad_P$ is a linear map from Hermitian or anti-Hermitian matrices into $su(n)$, $[\rho_1, P] = 0$ means that $P$ and $H_0$ have the same eigenstates. For the target state $\rho_f = |\psi_f\rangle\langle\psi_f|$ being a superposition state, in order to make the target state contain in $\mathcal{R}_1 \equiv \{ \rho_1 : [\rho_1, P] = 0 \}$, $P$ can be designed as

$$P = P_1|\psi_f\rangle\langle\psi_f| + \sum_{k=2}^n P_k |\psi_k\rangle\langle\psi_k|, \quad (31)$$

where $|\psi_1\rangle = |\psi_f\rangle$ and $\langle\psi_1|\psi_j\rangle = 0$, for $i \neq j$.

Then some deduction shows that $\rho_1 = \lambda_1|\psi_1\rangle\langle\psi_1|\lambda_1 = 1$. In order to make the system converge to the target superposition state $\rho_f$ from any initial pure state, one can design $P$ such that

$$V_S(\rho_f) < V_S(\rho_0) < V_S(\rho_{oth}), \quad (32)$$

where $\rho_{oth}$ represents any other state in the set $\mathcal{R}_1$ except the target state $\rho_f$.

For the satisfaction of $V_S(\rho_f) < V_S(\rho_{oth})$, one can design $P$ based on Proposition 6. In order to make (32) holds, one must design $P_i, (i = 1, \ldots, N)$ such that

$$0 < P_1 < P_1 \text{tr}(\rho_f \rho_0) + \sum_{k=2}^N P_k \text{tr}(\rho_k \rho_0) < P_j (j \neq 1). \quad (33)$$

However, for any initial pure state the target superposition state, there may not exist a $P$ such that (33) holds.

In conclusion, the design principle of $P$ for the case that the target state $\rho_f = |\psi_f\rangle\langle\psi_f|$ being a superposition state is (31), (33), and Proposition 6. We can also conclude that if the control system satisfies the conditions (i) and (ii) in Theorem 7 and there exists a $P$ to make (33) hold, any state trajectory of the system will converge to the target superposition state $\rho_f$ from any initial pure state $\rho_0$.

**Remark 8.** One can also solve the problem of the convergence of the control system governed by (1) to the target superposition state by means of designing the control laws in the interaction picture of the control system.

2.4. **Target Mixed State Which Does Not Commute with the Internal Hamiltonian.** From Sections 2.2 and 2.3, one can see that the control method proposed in Section 2.2 cannot guarantee the convergence to the target state which does not commute with the internal Hamiltonian. For the target state $\rho_f$ being a mixed state which does not commute with the internal Hamiltonian, that is, $[\rho_f, H_0] \neq 0$, Cong, Liu, and Yang proposed the control system in the interaction picture and used a unitary transformation to solve the convergence of the control system to the target state.

The basic idea is to use a unitary transformation $\hat{\rho}_f = U_f|\rho_f\rangle\langle\rho_f|U_f$ to make $[\hat{\rho}_f, H_0] = 0$ hold. Correspondingly, the control system governed by (28) after this unitary transformation will become

$$ih\hat{\rho}(t) = \sum_{k=1}^r \hat{H}_k(t) u_k(t) \hat{\rho}(t) \hat{\rho}(t), \quad (34)$$

where $\hat{\rho} = U_f|\rho_f\rangle\langle\rho_f|U_f$, $\hat{H}_k(t) = U_f^\dagger H_k(t)U_f$.

Then control laws can be designed according to Section 2.3. The research results show that the designed control laws and Theorem 7 are also valid with every physical quantity changing accordingly. In order to make $\hat{\rho}_f$ contain in $\mathcal{R}_2 \equiv \{ \hat{\rho}_f : [\hat{\rho}_f, P] = 0 \}$, $P$ needs to be designed such that $[H_0, P] = 0$ holds, $[\hat{\rho}_f, P] = 0$ and $[H_0, P] = 0$ imply that $\hat{\rho}_f, P,$ and $H_0$ have the same eigenstates. Since the evolution of $\hat{\rho}_f$ is unitary, all the $\rho_f(t)$ for $t \geq 0$ are isospectral. So the eigenvalues of $\hat{\rho}_f$ are a permutation of the eigenvalues of $\rho_f$. Thus the limit set $\mathcal{R}_2 \equiv \{ \hat{\rho}_f : [\hat{\rho}_f, P] = 0 \}$ has countable elements. For sake of the convergence from any initial mixed state $\rho_0$ to any target mixed state $\rho_f$ which does not commute with the internal Hamiltonian $H_0$, $P$ needs to be designed such that

$$V_S(\hat{\rho}_f) < V_S(\rho_0) < V_S(\rho_{oth}), \quad (35)$$

where $\rho_{oth}$ represents any other state in the set $\mathcal{R}_2 \equiv \{ \hat{\rho}_f : [\hat{\rho}_f, P] = 0 \}$ except $\hat{\rho}_f$.

In such a way, if there exists a $P$ to make (35) hold, any state trajectory of the system will converge to the target mixed state $\rho_f$ which does not commute with the internal Hamiltonian from any initial mixed state $\rho_0$.

Next, let us analyze how to make the restriction defined by (35) hold. Some deductions show that if one designs $P$ based on Proposition 6 with changing $\rho_f$ into $\hat{\rho}_f$ accordingly, then $V_S(\hat{\rho}_f) < V_S(\rho_{oth})$ will hold. Assume $\rho_0 = U\rho_f U^\dagger$. In order
to make the whole restriction defined by (35) hold, $P_i, (i = 1, \ldots, N)$ needs to be designed such that

$$(P)_{ii} > \left( \sum_{j \neq i} (P)_{ij} \sum_{j \neq k} \left( (\bar{\rho}_j)_{jj} - (\bar{\rho}_f)_{kk} \right) (U)_{ij} \right)^2 + (P)_{ii} \sum_{j \neq k \neq l} \left( (\bar{\rho}_j)_{jj} - (\bar{\rho}_f)_{kk} \right) (U)_{lj} \right)^2 \times \left( (\bar{\rho}_f)_{kk} - (\bar{\rho}_f)_{jj} \right)^{-1},$$

where $U_{ij}$ is the $(i, j)$th element of $U$.

In conclusion, the design principle of $P$ for the case that the target state is a mixed state which does not commute with $H_0$ is

(i) $P_i \neq P_m$ for any $i \neq m \in \{1, 2, \ldots, N\}$;

(ii) Proposition 6 with changing $\rho_f$ into $\bar{\rho}_f$;

(iii) Equations (36) and (16).

We can conclude from the above analysis that for the case that the target state is a mixed state which does not commute with $H_0$, if the control system is strongly regular and full connected, and one can seek an imaginary mechanical quantity $P$ to make (36) hold, then the control system can converge from any initial mixed state to the target mixed state which does not commute with the internal Hamiltonian.

3. Degenerate Cases

The convergence conditions (i) and (ii) proposed in the Theorem 1 through Theorem 7 are relevant to the internal Hamiltonian $H_0$ and the control Hamiltonians $H_k, (k = 1, \ldots, r)$. They are system parameters which cannot be changed. And in practice, many actual systems do not satisfy these convergence conditions. These systems are called in the degenerate cases. In order to solve the convergence of the control systems in degenerate cases, the existing method is to introduce a series of implicit function perturbations into the control laws and choose a Lyapunov function which is an implicit function [37–40].

In this section, we also divide the target state into four categories as: target eigenstate, the target mixed state which commute with the internal Hamiltonian, target superposition state, and the target mixed state which does not commute with the internal Hamiltonian. For these four target state categories, respectively, research results for the degenerate cases are summarized and analyzed.

3.1. Target Eigenstate. In this Section, the convergence of the control system based on the Lyapunov control method in the degenerate cases to any target eigenstate from any initial pure state will be summarized and analyzed.

3.1.1. Implicit Lyapunov Control Based on State Distance. In order to solve the convergence of the control systems in the degenerate cases, several researchers introduced a series of implicit function perturbations into the control laws [37–40]. After a series of perturbations $\gamma_k(t)$ introducing into the control laws, the dynamical equation (1) becomes

$$i |\psi(t)\rangle = \left( H_0 + \sum_{k=1}^{r} H_k (\gamma_k(t) + \nu_k(t)) \right) |\psi(t)\rangle,$$

where $\gamma_k(t) + \nu_k(t) = \varpi_k(t), (k = 1, \ldots, r)$ are the total control laws.

Without loss of generality, assume $|\psi_f\rangle = |\phi_f\rangle, 1 \leq g \leq N$. In order to solve the problem of convergence for the degenerate cases, the perturbations $\gamma_k(t)$ were introduced into the control laws. The basic idea is as follows: Denote the system with the internal Hamiltonian $H_0$, the control Hamiltonians $H_k, (k = 1, \ldots, r)$, and the control laws $\varpi_k(t) = \gamma_k(t) + \nu_k(t)$ as system 1, and the system with the internal Hamiltonian $H_{02} = H_0 + \sum_{k=1}^{r} H_k \varpi_k(t)$, the control Hamiltonians $H_k, (k = 1, \ldots, r)$, and the control laws $\varpi_k(t)$ as system 2. All these two systems can be depicted by (37). Denote the eigenvalues and eigenstates of $H_{02}$ as $\lambda_{1,\gamma_1(t)\ldots\gamma_r(t)}, \lambda_{2,\gamma_1(t)\ldots\gamma_r(t)}, \ldots, \lambda_{N,\gamma_1(t)\ldots\gamma_r(t)}$ and $|\phi_{1,\gamma_1(t)\ldots\gamma_r(t)}\rangle, |\phi_{2,\gamma_1(t)\ldots\gamma_r(t)}\rangle, \ldots, |\phi_{N,\gamma_1(t)\ldots\gamma_r(t)}\rangle$, respectively, which are the functions of the perturbations $\gamma_k(t)$. Assume $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle = |\phi_{g,\gamma_1(t)\ldots\gamma_r(t)}\rangle$. If one can design the perturbations $\gamma_k(t)$ such that (i) $\omega_{m,\gamma_1(t)\ldots\gamma_r(t)} \neq \omega_{l,\gamma_1(t)\ldots\gamma_r(t)}, (l, m) \neq (i, j), i, j, l, m \in \{1, 2, \ldots, N\}$, where $\omega_{m,\gamma_1(t)\ldots\gamma_r(t)} = \lambda_{m,\gamma_1(t)\ldots\gamma_r(t)} - \lambda_{\gamma_1(t)\ldots\gamma_r(t)}$, holds; (ii) for any $|\phi_{g,\gamma_1(t)\ldots\gamma_r(t)}\rangle \neq |\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$, there exists at least a $k \in \{1, \ldots, r\}$ satisfying $\langle \phi_{g,\gamma_1(t)\ldots\gamma_r(t)} | H_k | \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} \rangle \neq 0$, and select the specific Lyapunov function based on the state distance as

$$V_6(t) = \frac{1}{2} \left( 1 - |\langle \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} | \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} \rangle |^2 \right).$$

Then according to Section 2.1.1, system 2 will converge to $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$. And when system 2 converge to $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$, if the perturbations $\gamma_k(t)$ at $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$ are designed to equal zero, then system 2 will become system 1, and $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$ will become $|\psi_f\rangle$. Then 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 2 converges to $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$ from the initial state $|\psi_0\rangle$, another one is $\gamma_k(t)$ converges 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 $\gamma_k(t), (k = 1, \ldots, r)$ converging to 0 must be slower than the speed at which system 2 converges toward $|\psi_{f,\gamma_1(t)\ldots\gamma_r(t)}\rangle$. For convenience, the control system in the following section means system 1.

The existing design method of $\gamma_k(t)$ is to design it to be a monotonically increasing functional of $V(t)$, that is,

$$\gamma_k(t) = \theta_k (V(t)) = \theta_k \left( \frac{1}{2} \left( 1 - \frac{1}{\langle \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} | \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} \rangle |^2 \right) \right),$$

$$\gamma_k(t) = \theta_k (V(t)) = \theta_k \left( \frac{1}{2} \left( 1 - \frac{1}{\langle \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} | \psi_{f,\gamma_1(t)\ldots\gamma_r(t)} \rangle |^2 \right) \right),$$

where the function $\theta_k(\cdot)$ satisfies $\theta_k(0) = 0, \theta_k(s) > 0$ and $\theta_k'(s) > 0$ for every $s > 0$ and $s$ is the independent variable of the function $\theta_k(\cdot)$. 

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The right side of (39) contains $|\psi_{f,y_1(\ldots),y_r(\ldots)}\rangle$ which is a functional of the perturbations $y_k(t), (k = 1, \ldots, r)$. One can see that the relation between $y_k$ and the time $t$ is defined by $r$ equations and cannot be expressed by an explicit expression, so $y_k$ is the implicit function of the time $t$. From (38) and (39), one can also see that the Lyapunov function $V_k$ is the implicit function of the time $t$. The existence of $y'_k(t)$ can be depicted by Lemma 9.

Lemma 9 (see [37, 40]). Let $\theta_k(0) \in C^\omega(R^+; [0, \gamma_{k}^*])$, $k = 1, \ldots, r$, $(\gamma_{k}^* \in R, \gamma_k^* > 0)$ satisfy $\theta_k(0) = 0, \theta_k(s) > 0, \theta_k'(s) > 0$ for every $s > 0$, $\|\theta_k\|_{\infty} < 1/C^*$, and $C^* = 1 + \max\{||\partial^2\theta_k(y_1, \ldots, y_r, t)||_{y_1=0, \ldots, y_r=0}\}; \gamma_k(0) \in [0, \gamma_k^*]$, where $y_{k0} = \gamma_k(0)$. Then for every state $|\psi\rangle \in S^{2N-1} = \{x \in C^N; \|x\| = 1\}$, there exists a unique $y_1, y_2, \ldots, y_r$ with $y_k \in C^\omega(y_k \in [0, \gamma_k^*]), (k = 1, \ldots, r)$ satisfying $y_k(t) = \theta_k((1/2)(1 - [(\psi | ψ_{f,y_1(\ldots),y_r(\ldots)}(\ldots)(\ldots)])^2)) \{k = 1, \ldots, r, y_k(|\psi\rangle) = 0\}$. By (38) and Lemma 9, one can see that for every state $|\psi\rangle \in S^{2N-1} = \{x \in C^N; \|x\| = 1\}$; there also exists a unique $V_k$.

Assume
\[
\frac{\partial}{\partial y_1}|\psi_{f,y_1(\ldots),y_r(\ldots)}\rangle = \frac{\partial}{\partial y_2}|\psi_{f,y_1(\ldots),y_r(\ldots)}\rangle = \ldots = \frac{\partial}{\partial y_r}|\psi_{f,y_1(\ldots),y_r(\ldots)}\rangle.
\]  
(40)

The first order time derivative of the Lyapunov function (38) is
\[
V_k = \frac{-\sum_{k=1}^r \theta_k(t) \mathcal{A}\left((|\psi | \psi_{f,y_1(\ldots),y_r(\ldots)}\rangle \langle \psi_{f,y_1(\ldots),y_r(\ldots)} | H_k |\psi\rangle\right)}{(1 + \mathcal{R}\left((|\psi | \psi_{f,y_1(\ldots),y_r(\ldots)}\rangle \langle \psi_{f,y_1(\ldots),y_r(\ldots)} | \partial^2\theta_k |\psi\rangle\right)\sum_{j=1}^r \theta_j')}.
\]  
(41)

In order to make $V_k(t) \leq 0$, one can design $y_k(t)$ such that $||\theta_j'||_{\infty} < 1/(rC^*)$ to make $1/(1 + \mathcal{R}(\langle \psi | \phi_{y_1(\ldots),y_r(\ldots)}\rangle \langle \psi_{f,y_1(\ldots),y_r(\ldots)} | \partial^2\theta_k |\psi\rangle\langle \psi_{f,y_1(\ldots),y_r(\ldots)} | \partial^2\theta_k |\psi\rangle\rangle) > 0$ hold and design $y_k(t)$ as
\[
y_k(t) = K_k f_k \left(\mathcal{A}\left(e^{i_j \langle \psi | \psi_{f,y_1(\ldots),y_r(\ldots)}\rangle \langle \psi_{f,y_1(\ldots),y_r(\ldots)} | H_k |\psi\rangle\right)\right),
\]  
(42)

where $K_k > 0$, and $y_k(t), (k = 1, \ldots, r)$ are monotonic functions through the coordinate origin and in the first quadrant and the third quadrant.

Based on the LaSalle invariance principle, the convergence of the control system governed by (37) can be depicted by Theorem 10.

Theorem 10 (see [37, 40]). Consider the control system (37) with control fields $u_k(t) = y'_k(t) + v_k(t)$, $y_k(t)$ defined in (39), Lemma 9 and $||\theta_j'||_{\infty} < 1/(rC^*)$, and $v_k(t)$ defined in (42). Assume that the target state $|\psi\rangle$ is an eigenstate of $H_k$. If the control system satisfies (i) $\omega_{y_1, y_2, \ldots, y_r} \neq \omega_{y_1, y_2, \ldots, y_r}, (l, m) \neq (i, j)$, $i, j, l, m \in \{1, 2, \ldots, N\}$, $\omega_{y_1, y_2, \ldots, y_r} = \lambda_{y_1, y_2, \ldots, y_r} - \lambda_{y_1, y_2, \ldots, y_r}$, where $\lambda_{y_1, y_2, \ldots, y_r}$ is an eigenvalue of $(H_0 + \sum_{k=1}^r H_k y_k)$, (ii) For any $|\phi_{y_1, y_2, \ldots, y_r}\rangle \neq |\psi_{f,y_1(\ldots),y_r(\ldots)}\rangle$, there exists at least a $k \in \{1, \ldots, r\}$ satisfying $(\phi_{y_1, y_2, \ldots, y_r}(H_k|\psi_{f,y_1(\ldots),y_r(\ldots)}\rangle \neq 0; then the largest invariant set is $S^{2N-1} \cap E_{\gamma}$, where $E_{\gamma} = \{\psi \in C^\omega | e^{i \theta} |\psi\rangle, \theta \in R\}$. And the control system will converge toward $|\psi_j\rangle e^{i \theta}, (\theta \in R)$. Conditions (i) and (ii) in Theorem 10 are associated with $H_0, H_k, (k = 1, \ldots, r)$ and $y_k(t)$. By designing appropriate $y_k(t)$, these two conditions can be satisfied in most cases. One can see that if one designs appropriate control laws $u_k(t) = y'_k(t) + v_k(t), (k = 1, \ldots, r)$ to make the conditions (i) and (ii) hold, the control system depicted by (37) can converge to the equivalent state of the target eigenstate $|\psi_j\rangle$ from any initial pure state.

3.1.2. Implicit Lyapunov Control Based on the State Error.

The basic idea of this method is similar to that of the state distance. In the Lyapunov control based on the state error, a global phase control item $\omega$ is added into the control system to facilitate the design of the control laws. Thus the control system can be depicted by
\[
i |\psi(t)\rangle = \left( H_0 + \sum_{k=1}^r H_k (y_k(t) + v_k(t)) + \omega I \right) |\psi(t)\rangle,
\]  
(43)

where $u_k(t) = y'_k(t) + v_k(t), (k = 1, \ldots, r)$ and $\omega$ is the control laws which need to design.

Consider the Lyapunov function based on the state error as
\[
V_{z}(t) = \frac{1}{2} \langle \psi - \psi_{f,y_1(\ldots),y_r(\ldots)} | \psi - \psi_{f,y_1(\ldots),y_r(\ldots)} \rangle.
\]  
(44)

Thus the implicit function perturbation $y_k(t)$ needs to be designed as
\[
y_k(t) = \theta_k(V(t)) = \theta_k \left(\frac{1}{2} \langle \psi - \psi_{f,y_1(\ldots),y_r(\ldots)} | \psi - \psi_{f,y_1(\ldots),y_r(\ldots)} \rangle\right),
\]  
(45)

where functions $\theta_k(\cdot)$ satisfy $\theta_k(0) = 0, \theta_k(s) > 0, \theta'_k(s) > 0$ for every $s > 0$.

The existence of $y_k(t)$ can be depicted by Lemma 11.

Lemma 11 (see [38, 39]). Let $\theta_k \in C^\omega(R^+; [0, \gamma_{k}^*]), k = 1, \ldots, r, (\gamma_{k}^* \in R, \gamma_k^* > 0)$ satisfy $\theta_k(0) = 0, \theta_k(s) > 0, \theta_k'(s) > 0$ for every $s > 0$, $||\theta_k\|_{\infty} < 1/(rC^*)$, and $C^* = 1 + \max\{||\partial^2 \theta_k(y_1, \ldots, y_r, t)||_{y_1=0, \ldots, y_r=0}\}; \gamma_k(0) \in [0, \gamma_k^*]$. Then for every state $|\psi\rangle \in S^{2N-1} = \{x \in C^N; \|x\| = 1\}$, there exists a unique $y_1, y_2, \ldots, y_r$ and $y_k \in C^\omega(y_k \in [0, \gamma_k^*]), (k = 1, \ldots, r)$ satisfying $y_k(|\psi\rangle) = \theta_k((1/2)(\psi - \psi_{f,y_1(\ldots),y_r(\ldots)} | \psi - \psi_{f,y_1(\ldots),y_r(\ldots)} \rangle), y_k(|\psi\rangle) = 0$. 

Assume (40) holds, the first order time derivative of the Lyapunov function (44) is

\[
\dot{V}_\gamma = -\left( \frac{1}{1 + \Re \left( \langle \frac{1}{\partial \gamma_k} | \psi \rangle \rangle \right) \sum_j \theta_j \right) \cdot \left( \lambda_{\gamma_{1-\gamma_{r}}} + \omega \right) \mathcal{F} \left( \left| \psi_{f_{y_{1-\gamma_{r}}}} \right| \psi \right) + \sum_k \mathcal{F} \left( \left| \psi_{f_{y_{1-\gamma_{r}}}} \right| H_k \left| \psi \right) \right) v_k(t) \right).
\]

(46)

In order to make \( \dot{V}_\gamma(t) \leq 0 \), \( \omega \) and \( \gamma_k(t) \) need to be designed as

\[
\omega = -\lambda_{\gamma_{1-\gamma_{r}}} + c_0 \mathcal{F} \left( \left| \psi_{f_{y_{1-\gamma_{r}}}} \right| \psi \right),
\]

(47)

\[
v_k(t) = K_k f_k \left( \mathcal{F} \left( \left| \psi_{f_{y_{1-\gamma_{r}}}} \right| H_k \left| \psi \right) \right) \right), \quad (k=1,...,r),
\]

(48)

where \( K_k > 0 \), \( c > 0 \), and \( \gamma_k = f_k(x_k) \), \( (k=0,1,...,r) \) are monotonic functions along the coordinate origin and in the first quadrant and the third quadrant.

Based on the LaSalle invariance principle, the convergence of the control system governed by (44) can be depicted by Theorem 12.

**Theorem 12** (see [38, 39]). Consider the control system (43) with control fields \( \gamma_k(t) \) designed in (45) and Lemma II, \( v_k(t) \) designed in (48), and \( \omega \) designed in (47). Assume that the target state \( |\psi_f\rangle \) is an eigenstate of \( H_0 \). If the control system satisfies (i) \( \omega_{j_{1-\gamma_{r}}}, \gamma_{j_{1-\gamma_{r}}}, (i,j) \neq (i,j) \), \( i,j,l,m \in \{1,2,\ldots,N\}, \omega_{j_{1-\gamma_{r}}} = \lambda_{j_{1-\gamma_{r}}}, \gamma_{j_{1-\gamma_{r}}} \), is the \( l \)th eigenvalue of \( H_0 = \sum_{k=1}^{r} H_k \left| \psi_{f_{y_{1-\gamma_{r}}}} \right| \rangle \rangle \), corresponding to the eigenvector \( |\psi_{f_{y_{1-\gamma_{r}}}} \rangle \rangle \); (ii) There is at least a \( k \in \{1,...,r\}, \Phi_{f_{y_{1-\gamma_{r}}}}(t) \neq \Psi_{f_{y_{1-\gamma_{r}}}}(t) \langle \langle \langle \left| \psi_{f_{y_{1-\gamma_{r}}}} \right| \psi \rangle \rangle \rangle \), \( \left| \psi_{f_{y_{1-\gamma_{r}}}} \rangle \rangle \right\rangle \); then the largest invariant set is \( S^{N-1} \cap \mathcal{E}_g \), where \( E_g = \langle \left| \psi \right| \rangle = \ell^{2} \langle \left| \psi_f \right| \rangle, \theta \in \mathbb{R} \). And the control system will converge toward the equivalent state of the target state: \( |\psi_f\rangle \rangle \langle \langle \langle \left| \psi \right| \rangle \rangle \rangle, (\theta \in \mathbb{R}) \).

By designing appropriate perturbations \( \gamma_k(t) \), conditions (i) and (ii) in Theorem 12 can be satisfied in most cases. From Theorem 12, one can see that if one design appropriate control laws \( u_k(t) = \gamma_k(t) + v_k(t) \), \( (k=1,...,r) \) and \( \omega \) to make the conditions (i) and (ii) in Theorem 12 hold, the control system depicted by (43) can converge to the equivalent state of the target eigenstate \( |\psi_f\rangle \rangle \) from any initial pure state.

### 3.1.3. Implicit Lyapunov Control Based on Average Value of an Imaginary Mechanical Quantity.

For the implicit Lyapunov control based on the average value of an imaginary mechanical quantity, one can consider the control system depicted by (37). In this control method, the introduced implicit function perturbations \( \gamma_k(t) \) mainly have two tasks. One task is to solve the convergent problem of the control system in the degenerate cases. The basic idea is similar to that of the state distance. Another one is to choose a similar restriction \( V(|\psi_f\rangle) < V(|\psi_{\text{theo}}\rangle) \), which can be satisfied for any initial state and any target state by designing the imaginary mechanical quantity. In order to ensure the system converge to the target state by adding \( V(|\psi_f\rangle) < V(|\psi_{\text{theo}}\rangle) \), we can design all the perturbations \( \gamma_k(t) = 0 \) hold for \( k = 1,...,r \) only at \( |\psi_f\rangle \), that is, (1) \( \gamma_k(|\psi_f\rangle) = 0, (k = 1,...,r) \), and (2) for \( |\psi\rangle \neq |\psi_f\rangle \), there exists at least one \( k \) such that \( \gamma_k(|\psi\rangle) \neq 0 \). For sake of completing these two tasks, we can design \( \gamma_k(t) \) as a monotonically increasing functional of \( V(t) \):

\[
\gamma_k(|\psi\rangle) = C_k \cdot \theta_k \left( V(|\psi\rangle) - V(|\psi_f\rangle) \right),
\]

(49)

where \( C_k \geq 0 \), and for \( k = 1,...,r \), there exists at least a \( C_k > 0 \), and the function \( \theta_k(\cdot) \) satisfies \( \theta_k(0) = 0, \theta_k(s) > 0 \) and \( \theta_k'(s) > 0 \) for every \( s > 0 \), \( s \) is the independent variable of the function \( \theta_k(\cdot) \).

The specific Lyapunov function based on the average value of an imaginary mechanical quantity can be selected as:

\[
V_{\text{S}}(|\psi\rangle) = \langle \psi | P_{y_{1-\gamma_{r}}} | \psi \rangle,
\]

(50)

where \( P_{y_{1-\gamma_{r}}} = f(y_1(t),...,y_r(t)) \) is a functional of \( \gamma_k(t) \) and positive definite.

The existence of \( \gamma_k(t) \) can be depicted by Lemma 13.

**Lemma 13.** If \( C_k = 0, \gamma_k(|\psi\rangle) = 0 \). Else if \( C_k > 0, \theta_k \in C^\infty(R^*;[0,\gamma_k^*]), k = 1,...,r, (\gamma_k^* \text{ is a positive constant}) \) satisfy \( \theta_k(0) = 0, \theta_k(s) > 0 \) and \( \theta_k'(s) > 0 \) for every \( s > 0 \), \( s \) is the independent variable of the function \( \theta_k(\cdot) \).

\[
V_{\text{S}}(|\psi\rangle) = \langle \psi | P_{y_{1-\gamma_{r}}} | \psi \rangle
\]

(51)

where \( \gamma_k(t) = \gamma(t) = \theta((|\psi_f| P_{y_f}|\psi\rangle - \langle \psi_f | P_{y_f} | \psi_f \rangle), k = k_1,...,k_m; \)

(52)

where \( \theta(\cdot) = \theta_{k_1}(\cdot) = \cdots = \theta_{k_m}(\cdot) \) and \( P_f \) are functionals of \( \gamma(t) \).

The time derivative of the selected Lyapunov function is

\[
\dot{V}_{\text{S}} = \sum_{k=1}^{r} i v_k(t) \langle \psi | H_{k},P_{y_f} | \psi \rangle \left( (1 + \theta') \left( \langle \psi_f | (\partial P_{y_f}/\partial y) | \psi_f \rangle \right) \right) \left( (1 - \theta') \left( \langle \psi | (\partial P_{y_f}/\partial y) | \psi \rangle - \langle \psi_f | (\partial P_{y_f}/\partial y) | \psi_f \rangle \right) \right).
\]

(53)

In order to ensure \( \dot{V}_{\text{S}}(t) \leq 0 \), \( v_k(t) \) can be designed as

\[
v_k(t) = -K_k f_k \left( \langle \psi_f | H_{k},P_{y_f} | \psi_f \rangle \right), (k = 1,...,r),
\]

(54)
where $K_k$ is a constant and $K_k > 0$, and $y_k = f_k(x_k), (k = 1, 2, \ldots, r)$ are monotonic increasing functions through the coordinate origin of the plane $x_k = y_k$.

Based on LaSalle's invariance principle, the convergence of the control system governed by (37) can be depicted by Theorem 14.

**Theorem 14.** Consider the control system governed by (37) with control fields $u_k(t) = y_k(t) + v_k(t), (k = 1, \ldots, r)$, where $y_k(t)$ is defined by Lemma 13 and (51) and $v_k(t)$ is defined by (53). If the control system satisfies (i) $\omega_{l,m}^i = \omega_{l,m}^j, \forall (i, j) \neq (l, m)$, (ii) $i, j, l, m \in \{1, 2, \ldots, N\}$, $\omega_{l,m}^i = \lambda_{l,y}^i - \lambda_{m,y}^i$, where $\lambda_{l,y}^i$ is the $i$th eigenvalue of $H_0 + \sum_{k=1}^N H_k y(t)$ corresponding to the eigenstate $|\phi_i^l,y\rangle$; (iii) for any $i \neq j$, $i, j \in \{1, 2, \ldots, N\}$, there exists at least one $k$ such that $(\tilde{H}_k)_{lm} \neq 0$, where $(\tilde{H}_k)_{lm}$ is the $(l,m)$th element of $\tilde{H}_k = U_k^\dagger H_k U_k$; (iv) $|\phi_i^l,y\rangle \neq \phi_{j,m,y}^l$, then any trajectory will converge toward $E_9 = \{|\psi_{\text{other}}^i\rangle\}$.

From Theorem 14, one can see that if the target state $|\psi_f\rangle$ is an eigenstate, $|\psi_f\rangle$ is contained in $E_9$. In order to make the system converge to the target eigenstate from any initial pure state $|\psi_0\rangle$, on the one hand, $P_f$ needs to be designed to make

$$V_9(|\psi_f\rangle) < V_9(|\psi_{\text{other}}\rangle) \quad (54)$$

hold, where $|\psi_{\text{other}}\rangle$ represents any other state in the set $E_9$ except the target state. On the other hand, because $\partial V/\partial V > 0$, $V \leq 0, \forall t \geq 0$ holds, when $v_i(t) = 0, y(t) = \overline{y} \neq 0$ holds for some time, we can design $y = \overline{y} - \alpha, (0 < \alpha < \overline{y})$ to make the state trajectory evolve but not stay in $E_9$ until $|\psi_f\rangle e^{\overline{y}t}$ is reached.

Next, let us analyze how to realize the convergence conditions in Theorem 14 and restriction defined by (54). By designing appropriate $y_k(t)$, conditions (i) and (ii) in Theorem 14 can be satisfied in most cases. In order to make condition (iii) be satisfied, the eigenvalues of $P_f$ can be designed constant, denoted by $P_1, P_2, \ldots, P_N$, and $P_f$ can be designed as

$$P_f = \sum_{j=1}^N P_j |\phi_j,f\rangle \langle \phi_{j,f}| \quad (55)$$

To make condition (iv) satisfied, $P_i \neq P_j, \forall i \neq j, 1 \leq i, j \leq N$ can be designed. The results on how to make (54) hold can be depicted by Theorem 15.

**Theorem 15.** If one designs $P_i > P_j, (i = 1, \ldots, N, P_i \neq P_j)$, then $V_9(|\psi_f\rangle) < V_9(|\psi_{\text{other}}\rangle)$ holds, where $P_f$ is the eigenvalue of $P_f(|\psi_f\rangle)$ corresponding to $|\psi_f\rangle$.

We can conclude from the above analyses that by using the implicit Lyapunov control based on the imaginary mechanical quantity, if one designs appropriate control laws $u_k(t) = y_k(t) + v_k(t), (k = 1, \ldots, r)$ to make the conditions (i)–(iv) in Theorem 15 and (54) hold, the control system governed by (37) in the degenerate cases can converge from any initial pure state to the target eigenstate. The design principle of the imaginary mechanical quantity $P_f$ is Theorem 15 and (55).

### 3.2. Target Superposition State

The method proposed in Section 3.1 cannot guarantee the control system governed by (37) or (43) in the degenerate cases converge from any initial pure state to the target superposition state. In order to solve this problem, one can introduce a series of constant disturbances $\eta_k$ into the control laws. Thus the mechanical equation (37) becomes

$$i |\psi(t)\rangle = \left( H_0 + \sum_{k=1}^r H_k (\eta_k + y_k(t) + v_k(t)) \right) |\psi(t)\rangle \quad (56)$$

And the mechanical equation (43) in Section 3.1.2 becomes

$$i |\psi(t)\rangle = \left( H_0 + \sum_{k=1}^r H_k (y_k(t) + v_k(t) + \eta_k) + \omega l \right) |\psi(t)\rangle \quad (57)$$

where $\eta_k \in R$.

The basic idea of solving the convergence to the target superposition state is to design $\eta_k$ 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 Hamiltonians $r$ is large enough, by designing appropriate $\eta_k, (H_0 + \sum_{k=1}^r H_k \eta_k) |\psi_f\rangle = \lambda_f |\psi_f\rangle$ can be satisfied in most cases, where $\lambda_f$ is the eigenvalue of $H_0 + \sum_{k=1}^r H_k \eta_k$ corresponding to $|\psi_f\rangle$. Then one can design the control laws and analyze the convergence according to the method for the target eigenstate cases. Research results show that every conclusion in Section 3.1 also holds with changing $H_0$ into $H_0'$

### 3.3. Target Mixed State Which Commutes with the Internal Hamiltonian

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

$$i \dot{\rho}(t) = \left[ H_0 + \sum_{k=1}^r H_k (y_k(t) + v_k(t)), \rho(t) \right] \quad (58)$$

where $y_k(t) + v_k(t) = u_k(t)$ are the total control laws.

The design ideas are similar to those of Section 3.1. Consider the Lyapunov function based on the imaginary mechanical quantity as

$$V_9(\rho) = \text{tr} \left( P_{y_i\cdots y_j}\rho \right) \quad (59)$$

$y_k(t)$ can be designed as

$$y_k(t) = \gamma(t) = \theta \left( V_9(\rho) - V_9(\rho_f) \right), \quad k = k_1, \ldots, k_m; \quad y_k(t) = 0, \quad k \neq k_1, \ldots, k_m (1 \leq k_1, \ldots, k_m \leq r). \quad (60)$$

The existence of $\gamma(t)$ can be depicted by Lemma 16.
Lemma 16. If $\theta \in C^\infty(R^s;[0,\gamma^*]), k = 1, \ldots, r$ ($\gamma^*$ is a positive constant) satisfy $\theta(0) = 0, \theta(s) > 0$ and $\theta'(s) > 0$ for every $s > 0$, and $|\theta'| < 1/(2C^*), C^* = 1 + C, C = \max\{||P_k||_m, \gamma \in [0,\gamma^*]\}$, then for every $\rho$, there is a unique $\gamma \in C^\infty([0,\gamma^*])$ satisfying $\gamma(\rho) = \theta(\text{tr}(P_\rho \rho - \text{tr}(P_\rho)))$.

According to the Lyapunov stability Theorem, $v_k(t)$ can be designed as

$$v_k(t) = K_k f_k \left( i \text{tr} \left( \left[ P_k, H_k \right] \rho \right) \right), \quad (k = 1, \ldots, r), \quad (61)$$

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

Based on the LaSalle invariance principle, the convergence of the control system can be depicted by Theorem 17.

Theorem 17. Consider the control system depicted by (58) with control laws $u_k(t) = y_k(t) + v_k(t)$, where $y_k(t)$ is defined by Lemma 16 and (60), and $v_k(t)$ is defined by (61). If the control system satisfies (i) $\omega_{m,n} \neq \omega_{i,j}, (i, j, m \neq i, j, n, m \in \{1, 2, ..., N\}, \omega_{m,n} = \lambda_{m,n}$, where $\lambda_{i,j}$ is the $i$th eigenvalue of $(H_0 + \sum_{k=1}^N \omega_{m,n} H_m y(t))$ corresponding to the eigenstate $|\phi_{i,j}\rangle$; (ii) $\forall j \neq i, \{k = 1, \ldots, r \}$, there exists at least a $(\hat{H}_k)_{ii} \neq 0$, where $(\hat{H}_k)_{ii}$ is the $(j,1)$th element of $(\hat{H}_k) = U_H^* H_k U_2$ with $U_2 = \{ |\phi_{1,y}\rangle, \ldots, |\phi_{N,y}\rangle \}$; (iii) $[P_{k'}, H_0 + \sum_{m=1}^N \omega_{m,k'} H_m y(t)] = 0, 1 \leq k_1, \ldots, k_m \leq r$; (iv) for any $l \neq j, (1 \leq l, j \leq N)$, $(\hat{H}_l)_{ii} \neq 0$, holds, where $(\hat{H}_l)_{ii}$ is the $(l,1)$th element of $(\hat{P}_y) = U_H^* P_{k'} U_2$, then the control system will converge toward $E_{10} = \rho_{10} \{(U_2^* P_{k'} U_2)_{ii} \}_{ii} = 0, y = \gamma(\rho_{10}), t_0 \in \mathbb{R}$.

For the target state $\rho_{10}$ which commutes with the internal Hamiltonian; that is, $[\rho_{10}, H_0] = 0$, $\rho_{10}$ is contained in $E_{10}$. In order to make the system converge to the target state $\rho_{10}$ which commutes with $H_0$ from any initial state; on the one hand, $P_y$ needs to be designed to make

$$V_9(\rho_{10}) < V_9(\rho_{\text{other}}) \quad (62)$$

hold, where $\rho_{\text{other}}$ represents any other state in the set $E_{10}$ except the target state. On the other hand, $y$ was designed as $y = \gamma - \alpha, (0 < \alpha \ll \gamma)$ when $v_k(t) = 0, \gamma(t) = \gamma \neq 0$ holds for some time to make the state trajectory evolve but not stay in $E_{10}$ until $\gamma_1$ is reached.

For the satisfaction of conditions (i)–(iv) in Theorem 17, one can follow that of Section 3.1.3. In order to make (62) hold, one can design $P_y$ based on Proposition 6. The total design principle of $P_y$ is (55) and Proposition 6.

We can conclude from the above analyses that for the target state which commutes with the internal Hamiltonian, by using the implicit Lyapunov control method based on the imaginary mechanical quantity, if one designs appropriate control laws $u_k(t) = y_k(t) + v_k(t), (k = 1, \ldots, r)$ to make the conditions (i)–(iv) in Theorem 17 and (62) hold, the control system governed by (58) in the degenerate cases can converge from any initial state to the target state which commutes with the internal Hamiltonian, which contains the target eigenstate and the target mixed state which commutes with the internal Hamiltonian.

3.4. Target Mixed State Which Does Not Commute with Internal Hamiltonian. For the target mixed state which does not commute with the internal Hamiltonian, the design idea is similar to Section 3.2. The difference is to design $\eta_0$ to make $[\rho_{10}, H_0'] = 0$. If the number of the control Hamiltonians $r$ is large enough, by designing appropriate $\eta_0, [\rho_{10}, H_0'] = 0$ can be satisfied in most cases. Then one can design the control laws and analyze the convergence according to the method mentioned in Section 3.3. Research results show that every conclusion in Section 3.3 also holds with changing $H_0$ into $H_0'$.

4. Conclusion

In this paper, for the non-degenerate and degenerate cases, the existing quantum Lyapunov control based on the state distance, state error, and average value of an imaginary mechanical quantity for the control systems have been summarized and analyzed. For the target state being the eigenstate, the mixed state which commutes with the internal Hamiltonian, the superposition state, and the mixed state which does not commute with the internal Hamiltonian, respectively, the design methods of the control laws have been summarized; the convergence to the target state has been summarized and analyzed. Research results show that the Lyapunov-based control method can make the control system converge from any initial state to the target state in both non-degenerate and degenerate cases. After ten years of development, the quantum control theory based on the Lyapunov stability theorem has been established.

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References


Research Article

High Sensitivity Optically Pumped Quantum Magnetometer

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Quantum magnetometers based on optical pumping can achieve sensitivity as high as what SQUID-based devices can attain. In this paper, we discuss the principle of operation and the optimal design of an optically pumped quantum magnetometer. The ultimate intrinsic sensitivity is calculated showing that optimal performance of the magnetometer is attained with an optical pump power of 20 μW and an operation temperature of 48°C. Results show that the ultimate intrinsic sensitivity of the quantum magnetometer that can be achieved is 327 fT/Hz$^{1/2}$ over a bandwidth of 26 Hz and that this sensitivity drops to 130 pT/Hz$^{1/2}$ in the presence of environmental noise. The quantum magnetometer is shown to be capable of detecting a sinusoidal magnetic field of amplitude as low as 15 pT oscillating at 25 Hz.

1. Introduction

Optically pumped quantum magnetometers are based on the use of the atomic-spin-dependent optical properties of a medium. The general principle of operation of optically pumped quantum magnetometers is described in detail in [1]. A circularly polarized laser light transmitted through a glass cell containing a vapor of alkali atoms (e.g., Cs) resonates when its frequency equals the first absorption line of the alkali atoms, thus creating a spin alignment that precesses with a frequency proportional to the modulus of an externally applied magnetic field, $B_0$ (Larmor frequency, $\omega_L = \gamma |B_0|$). If this precession is coherently driven by an rf magnetic field, $B_{rf}$ (oscillating at frequency $\omega_{rf}$), the absorption coefficient of the alkali medium changes, thus modulating the transmitted optical intensity. By applying a very small oscillating magnetic field and maintaining the driving rf magnetic field resonant with the Larmor frequency, that is, $\omega_{rf} = \omega_L$, the very small oscillating magnetic field can be determined. Several optical magnetometers have been developed, demonstrating sensitivities as high as those of superconducting quantum interference device- (SQUID-) based magnetometers. However, SQUID-based magnetometers must be operated at very low temperatures, thus requiring expensive cooling mechanisms. On the other hand, optical magnetometers not only work at room temperature but also have the potential of miniaturization, making them more practical for many applications [2, 3].

The basic operation mode of optical magnetometers involves the following mechanisms: Coherent Population Trapping (CPT), Nonlinear-Magneto Optical Rotation (NMOR), Spin-Exchange Relaxation Free (SERF) regime, and Mx magnetometer. The CPT method is an all-optical technique based on the use of two light sources (probe and pump) with orthogonal polarizations that create a coupling between two Zeeman sublevels located in different hyperfine states. When the modulation of the probe light is in resonance with the Zeeman splitting frequency ground sublevels a decrement in the light intensity can be observed. CPT-based magnetometers work in a scalar mode. The application of CPT-based magnetometers to cardiosignal detection has been demonstrated showing a sensitivity of 1 pT/Hz$^{1/2}$ in an unshielded environment [4].

The NMOR technique is based on the linear magneto optical (Faraday) rotation principle. When the light modifies the properties of the medium, a nonlinear magneto optical rotation occurs. This happens when the light frequency is resonant with the atomic transitions of the medium, thus allowing the optical absorption to take place. The dynamic range of an NMOR-based magnetometer is limited by the width of the resonance, and the sensitivity that can be
obtained experimental results. Described finally in Section 4, we represent and discuss the obtained experimental results.

Section 2, we explain the principle of operation of an optical Mx magnetometer and demonstrate experimentally the dependence of its sensitivity and bandwidth upon the light power and the frequency. This kind of optical magnetometers can reach a sensitivity of 0.15 pT/Hz\(^{1/2}\) [5], which is adequate for geomagnetic measurements. The magnetometers operating in the SERF regime are also based on NMOR principle. However, such magnetometers have limited sensitivities due to depolarization caused by various atoms interaction types. The dominant type of these interactions is the spin-exchange collisions that can change the hyperfine state of the atoms while preserving the total angular momentum of the colliding atom pair. This results in a dephasing of the atom ensemble in the presence of a magnetic field, which makes the measurement of the Larmor frequency difficult. However, decoherence due to spin-exchange collisions can be completely eliminated if the spin-exchange collisions occur faster than the precession frequency of the atoms. This kind of optical magnetometers can reach a sensitivity of 0.54 fT/Hz\(^{1/2}\) [6]. The Mx magnetometers are so called because an rf oscillating magnetic field is supplied to the atoms to modulate the x-component of the magnetization vector inside the vapor cell. The phase difference between the driving rf signal and the probe light transmitted through the vapor cell gives a direct measurement of the Larmor frequency. This kind of magnetometer is vastly used in magnetocardiography, and it can reach sensitivity of 99 fT/Hz [7]. Optical magnetometers based on CPT and SERF regime operate in zero-magnetic-field conditions while the others require a weak magnetic field to induce Zeeman splitting. Between all the operation modes of optical magnetometers, the Mx configuration and SERF regime can achieve the highest sensitivity. An attractive feature of magnetometers working in the SERF regime is that they do not need an rf magnetic field or magnetic coils in the proximity of the vapor cell, which could create crosstalk problems in array configurations. On the other hand, the SERF regime requires higher temperature to attain high sensitivity and only works in very weak magnetic fields because the frequency of collisions must be higher than the Larmor frequency. This makes the SERF regime much more susceptible to environmental noise.

In this paper, we describe the principle of operation of an Mx-configuration-based optically pumped quantum magnetometer and demonstrate experimentally the dependence of its sensitivity and bandwidth upon the light power and the alkali vapor temperature. The paper is organized as follows. In Section 2, we explain the principle of operation of an optical Mx magnetometer. In Section 3, the experimental setup is described. Finally in Section 4, we present and discuss the obtained experimental results.

2. Atomic Mx Magnetometer

The generic configuration of an optical Mx magnetometer is shown in Figure 1. The core of the system is a glass cell filled with the vapor of one of the alkali metals that have only one electron in their outermost shell. Generally, cesium is used because it possesses only one stable isotope, \(^{133}\text{Cs}\), with a nuclear spin \(I = 7/2\).

When a uniform dc external magnetic field is applied, each hyperfine level of cesium atoms splits into \(2F+1\) Zeeman sublevels, as displayed in Figure 2. The light source is used both for pumping the Cs atoms to excited states and as a probe signal that senses an rf oscillating magnetic field modulating the absorption coefficient of the Cs atoms. Photons having a wavelength equal to the first absorption line of the alkali atoms are absorbed by the cesium atoms, thus moving them to the excited state. Figure 2 shows the optical pumping over the \(F = 4 \rightarrow F = 3\) transition of the cesium D1 absorption line using right circularly polarized light, which results in photon's angular momentum equal to +1. A Cs atom in the lower state with a quantum number \(m_F\) is allowed to move only to the upper level with \(m_F' = m_F + 1\) because of total angular momentum conservation. A Cs atom that is in the excited state can decay via one of three possible decay channels and it spontaneously emits a photon that has equal probability to be sent in any direction, not necessary the direction of light beam. Therefore, there is a finite probability for the atom to decay into a level with a larger \(m_F\) value; thus, if the pumping process is repeated several times the atom moves to the two outermost states \((m_F = 3\) and 4) and, eventually, can no longer be optically pumped because there is not a corresponding state in the excited level available for transition [8]. Since these atoms do not absorb light, they are called dark states.

The Cs atoms in the dark states precess around the magnetic field axis at the Larmor frequency that is proportional to the field magnitude: \(\omega_L = \gamma |B_0|\), where \(\gamma\) is the gyromagnetic constant that for cesium is \(2\pi \cdot 3.5\) Hz/nT. During this time, the atom spin accumulates an increasing phase angle.

![Figure 1: The generic configuration of an optical Mx magnetometer.](image1)

![Figure 2: Fine, hyperfine structures and Zeeman splitting of the cesium D1 line with the optical pumping process and the dark states highlighted.](image2)
The spin state of an atom can be changed to an absorbing (nondark) state through the absorption of resonant radio frequency radiation. A change in the spin orientation causes a Cs atom to come out of the dark state into an absorbing state. Amplitude modulation of the transmitted light can be achieved when a large fraction of the atoms precess coherently in phase [9]. To maintain this coherence and synchronize the precession of atomic spins, the rf driving magnetic field must be resonant with the Larmor frequency, that is, \( \omega_{rf} = \omega_z \). The ensemble average of the magnetic moments associated with the spins can be treated as a classical magnetization vector \( M \). The precession of \( M \) around the total (dc and ac) magnetic field \( (B_{tot} = zB_0 + xB_{1z} \cos(\omega_{1z}t)) \) is given by the Bloch equations [10]:

\[
\begin{pmatrix}
\dot{M}_x \\
\dot{M}_y \\
\dot{M}_z
\end{pmatrix}
= \begin{pmatrix}
M_x \\
M_y \\
M_z
\end{pmatrix} \times \begin{pmatrix}
\gamma B_{1z} \cos(\omega_{1z}t) \\
0 \\
\gamma B_0
\end{pmatrix} - \begin{pmatrix}
\Gamma_2 M_x \\
\Gamma_2 M_y \\
\Gamma_1 M_z
\end{pmatrix},
\]

where \( \Gamma_1 \) and \( \Gamma_2 \) are the longitudinal and the transverse relaxation time, respectively. The calculated in-phase and quadrature amplitudes and the phase shift of light power with respect to the driving rf magnetic field, \( B_{1z} \), are given by

\[
\begin{align*}
P_{in} (\delta) &= -P_0 \sin(2\theta) \frac{\Omega_{1z}^2 \delta}{\Omega_{1z}^2 \Gamma_2 / \Gamma_1 + \Gamma_2^2 + \delta^2}; \\
P_{qu} (\delta) &= -P_0 \sin(2\theta) \frac{\Omega_{1z} \Gamma_2}{\Omega_{1z}^2 \Gamma_2 / \Gamma_1 + \Gamma_2^2 + \delta^2}; \\
\phi &= \arctan \frac{\Gamma_2}{\delta},
\end{align*}
\]

where \( \Omega_{1z} = \gamma \cdot \omega_{1z} \) is the Rabi frequency, \( \delta = \omega_{1z} - \omega_z \) is the frequency detuning from the Larmor frequency, and \( \theta \) is the angle between the laser beam and \( B_z \).

Several important parameters can affect the magnetometer sensitivity, namely, the laser power; the laser beam profile, the rf field power, the cell size, the buffer-gas pressure, and the density of Cs atoms (which depends on the temperature). Typically, the magnetometer spatial resolution depends on the cell dimensions. In this paper, we focus the investigation on the effects of optical power intensity and vapor cell temperature variations on the sensitivity and bandwidth of the optical Mx magnetometer.

3. Experimental Setup

The Mx magnetometer used in the experiment is shown in Figures 3(a) and 3(b). The core of the instrument is a quartz-made cylindrical cell containing Cesium vapor. Also, Neon at 34 Torr and Argon at 6 Torr are added to the Cs vapor in order to reduce atom collisions. The cell diameter and length are 21 mm and 75 mm, respectively, yielding a spatial resolution of about 53 mm. In the experiments, the gas pressure inside the cell was increased by increasing the temperature using hot water flowing into a silicon pipe wrapped around the cell. The vapor cell was placed in the center of an electromagnet that generates a dc magnetic field in order to cancel the geomagnetic field and supply a uniform magnetization along the appropriate direction inside the vapor cell. The used electromagnet consists of two parts: (i) a 3D DC coils of dimension 580 mm × 530 mm × 640 mm providing a magnetic field with a uniformity better than 1% in the central region and (ii) an additional pair of coils that generate a small-magnitude rf magnetic field along the x-axis. Each coil pair of the electromagnet was independently driven by a digital power supply to cancel the geomagnetic field along the x- and y-directions and generate a uniform magnetic field along the z axis. The intensity of the magnetic field at the center of the electromagnet was 13 μT, as measured by a three-axis smart digital magnetometer Honeywell HMR2300. The AC coils were driven by a waveform generator (Agilent, model 33250A) to produce an rf magnetic field of intensity 200 nT, oscillating at 45.5 kHz along the x-axis.

An external-cavity semiconductor laser (made by Uni-quanta Technology, Beijing, China) was used as light source for both pumping and probing. The laser wavelength was tuned to 894 nm which is equal the cesium D1 absorption line \( F = 4 \rightarrow F = 3 \) transition and stabilized using saturation spectroscopy in an auxiliary cell. The frequency stabilized light was coupled into a single-mode polarization...
maintaining optical fiber of 5 µm core diameter and delivered
to the vapor cell which was placed inside the electromagnet. At
the cell location, the light was collimated, providing an output beam diameter of 1.6 mm, and right circularly polarized using a half-wave plate, an optical polarizer, and a
carrier-wave plate. The laser beam was transmitted through the vapor cell at an angle of 45 degrees with respect to both
the z- and the x-axes. The output light beam was focused into
a photodiode (PED801 from UniQuanta Technology), which
was placed outside the electromagnet in order to reduce the magnetic interference produced by the transimpedance amplifier of the photodiode package. A spectrum analyzer (Agilent, model E4407B) was used to measure the power spectral density of the photodiode output in order to calculate the signal-to-noise ratio and hence the intrinsic and actual sensitivity of the optical Mx magnetometer. Finally, a lock-
in amplifier (Stanford Research Systems, model SR530) was used to measure the phase shift between the photocurrent detected by the photodiode with respect to the oscillating rf magnetic field, and the in-phase component and
the quadrature component. Note that, by sweeping the frequency of the rf magnetic field along the Larmor frequency, the half width at half maximum (HWHM) of the in-phase, the quadrature and the phase signals could be measured.

It is important to mention that all the experimental results reported below were performed in laboratory environment
without any magnetic shield. The uniform magnetic field along the z-axis was 13 µT corresponding of a Larmor frequency of 45.5 kHz. It is also important to note that when the measurements were carried out with different uniform dc magnetic field intensities the performances of the magnetometer were not affected. The intensity of the rf magnetic field was 200 nT. In the experiments, the optical Mx magnetometer was operated in free-running mode without
the use of a feedback loop between the lock-in amplifier and the signal generator to lock the rf frequency to the Larmor frequency. Particularly, the dependence of the sensitivity and the bandwidth of the optical Mx magnetometer on cell temperature and optical power was investigated for different input optical power levels over a cell temperature range of 23°C to 55°C.

4. Results and Discussion

4.1. Sensitivity. The sensitivity of the optical Mx magnetome-
ter is defined as the smallest change in magnetic field that
can be detected by the magnetometer. The sensitivity can be
calculated using the Cramer-Rao equation [11]:

\[ \rho = 4\sqrt{3} \sqrt{f_{bw}} / \gamma \text{SNR}, \]

where \( f_{bw} \) is the bandwidth, \( \gamma \) is the gyromagnetic constant and SNR is the signal-to-noise ratio of the magnetometer. All the following results refer to a 1 Hz bandwidth.

The SNR can be calculated from the measured power spectral density (PSD) of the photodiode output, as illustrated in Figure 4. Since the magnetometer was operated
in a magnetically-unshielded environment, all the measure-
ments were dominated by the magnetic field noise.

The intrinsic signal-to-noise ratio was calculated with the
noise being the intrinsic rms noise of the magnetometer, measured over 100 Hz from the resonance frequency. The actual signal-to-noise ratio was calculated by taking into account the sidebands induced by the 50 Hz magnetic noise produced by power lines. Figure 5 shows the intrinsic SNR (a) and the intrinsic sensitivity (b) of the magnetometer versus the cell temperature for different input optical power levels.

The intrinsic SNR, and hence the intrinsic sensitivity, curve exhibits a similar trend for all input optical power levels, namely, the SNR increases with increasing temper-
are, reaching a maximum value around 50°C before it starts to decrease. Moreover, increasing the input optical power increases the intrinsic SNR, and hence the intrinsic sensitivity. In fact, when the temperature increases, the gas pressure inside the vapor cell increases, resulting in a higher number of atoms interacting with the light and coherently precessing around the magnetic field at the Larmor frequency. Furthermore, increasing the input optical power results in a greater number of atoms being optically pumped. However, when the gas pressure is too high, the collisions of atoms with each other or with the walls of the cell lead to phase incoherence during precession, thus reducing the SNR performance of the magnetometer. The best performance of the magnetometer was obtained with an input optical power of 20 µW and a cell temperature of 50°C. The measured
intrinsic SNR was 5000 and the intrinsic sensitivity was
63 fT/Hz\(^{1/2} \), measured in a 1 Hz bandwidth.

To obtain the actual SNR and the actual sensitivity of the
magnetometer, the SNR was calculated by taking into account
the external magnetic noise. Obviously, the actual sensitivity is strongly dependent on the location of the magnetometer. All the experiments reported in this paper were performed in the laboratory environment without any magnetic shield. This resulted in a very poor actual signal-to-noise ratio, and hence, a very low actual sensitivity. Figures 6(a) and

![Figure 4: Power spectral density of the photodiode output normalized to the resonance frequency. The spectrum was measured in a 1 Hz bandwidth. The signal was recorded with optical power of 20 µW and cell temperature of 50°C. The intrinsic and actual signal-to-noise ratios are highlighted.](image)
Figure 5: (a) Intrinsic signal-to-noise ratio (SNR) and (b) intrinsic sensitivity, measured in a 1 Hz bandwidth versus cell temperature for input optical power of 10 $\mu$W, 15 $\mu$W, and 20 $\mu$W.

Figure 6: (a) Actual signal-to-noise ratio (SNR) and (b) actual sensitivity versus cell temperature, measured in a 1 Hz bandwidth for an input optical light power of 10 $\mu$W, 15 $\mu$W, and 20 $\mu$W.
show the actual SNR and the actual sensitivity of the magnetometer, respectively. Also noticed in this case that the actual SNR increases (and hence the actual sensitivity is enhanced) with increasing the input optical power. However, the actual SNR decreases with increasing the cell temperature, mainly because of the higher phase incoherence that reduces the output signal level. With an input optical power of 20 μW and a cell temperature of 50°C, the actual SNR dropped to 11.6 and the actual sensitivity was 27 pT/Hz\(^{1/2}\), measured in a 1 Hz bandwidth. The best actual sensitivity was obtained with an input optical power of 20 μW at room temperature (23°C). The corresponding actual SNR was 14.5 and the actual sensitivity was 21 pT/Hz\(^{1/2}\), measured in a 1 Hz bandwidth.

4.2. Bandwidth. Another important feature of a magnetometer is its bandwidth, that is, how fast the magnetometer responds to changes in the magnetic field. The bandwidth, \(f_{bw}\), of the magnetometer can be calculated as [12]:

\[
f_{bw} = \frac{\pi}{2} \Delta \nu,
\]

where \(\Delta \nu\) is the half width at half maximum (HWHM) bandwidth of the phase signal measured in hertz, as illustrated in Figure 7(c).

Figures 7(a) and 7(b) show, respectively, the in-phase and quadrature components of the lock-in amplifier output versus the normalized frequency, predicted by (2) and (3). Figure 7(c) shows the phase shift between the photodiode output and the driving rf magnetic field, \(B_{rf}\), predicted by (4). All signals in Figures 7(a)–7(c) were measured in a magnetically unshielded environment by continuously sweeping the driving rf frequency along the resonance frequency over a 6-second time range. It is important to note that the magnetically induced 50 Hz interference signal was suppressed by a notch filter. It is obvious from Figures 7(a)–7(c) that the HWHM bandwidths of both the in-phase signal, \(\Delta \nu_X\), and the quadrature signal, \(\Delta \nu_Y\), are equal and smaller than the HWHM bandwidth, \(\Delta \nu\), of the phase-shift signal. This agrees with the theoretical prediction using (2)–(4). In fact, the phase shift is the only signal that is not dependent on the rf magnetic field. Therefore, for the accurate evaluation of the bandwidth of the magnetometer, \(f_{bw}\), it is important to use into (6) the HWHM bandwidth, \(\Delta \nu\), measured from the phase shift rather than the HWHM bandwidths, \(\Delta \nu_X\) and \(\Delta \nu_Y\), measured from the in-phase and quadrature components, respectively.

Figure 8 shows the magnetometer bandwidth versus cell temperature for input optical power levels of 10 μW, 15 μW, and 20 μW. The bandwidth exhibits a similar trend for all input optical power levels, initially decreasing with increasing the cell temperature until reaching its minimum around 45°C. Subsequently the bandwidth increases with increasing the cell temperature. The bandwidth depends on the transverse relaxation time \(T_2\), as evident from (4) and (6). An increase in the cell temperature increases the vapor pressure, which results in a larger number of atoms interacting with the light, leading to a longer relaxation time (smaller bandwidth). However, at high temperature, the number of collisions between atoms or with the walls of the cell increases significantly, leading to a shorter relaxation time and hence a larger bandwidth. This explains the existence of a critical temperature (around 45°) at which the intrinsic bandwidth is minimum.

In the experiments, the measured maximum bandwidth was 175 Hz, obtained at room temperature (23°C) with an input optical power of 10 μW (blue curve in Figure 8), while the minimum bandwidth was 25 Hz, obtained with an input optical power of 20 μW at a temperature of 45°C (black curve in Figure 8).

4.3. Low-Amplitude Magnetic Field Measurement. The ultimate intrinsic sensitivity of the magnetometer can be calculated using (5). The best performance of the magnetometer was obtained for an input optical power of 20 μW at cell temperature of 48°C; the ultimate intrinsic sensitivity was 327 fT/Hz\(^{1/2}\) over a bandwidth of 26 Hz. However, the external magnetic noise generated by power lines and surrounding equipment caused the actual ultimate sensitivity of the
magnetometer to drop to 130 pT/Hz\(^{1/2}\) over a bandwidth of 26 Hz.

The magnetometer in its optimal configuration (input optical power of 20 \(\mu\)W at cell temperature of 48°C) was then used to measure an applied small-signal sinusoidal magnetic field of amplitude 15 pT oscillating at 25 Hz, which was generated by a test coil placed at a distance of 6 cm from the vapor cell. For this measurement, the uniform dc magnetic field was 13 \(\mu\)T, corresponding to a Larmor frequency of 45.5 kHz. The frequency of the rf magnetic field was then set at 45.5 kHz resulting in a phase shift of -90 degrees between the photodiode output and the driving rf signal, as predicted by (4), and verified experimentally by the result shown in Figure 7(c). When another 25 Hz small-amplitude magnetic field was applied in addition to the dc and rf magnetic fields, the Larmor frequency changed and no more resonance occurred, causing the phase shift between the photodiode output and the driving rf signal to oscillate around -90 degrees at 25 Hz. This enabled the measurement of the new Larmor frequency and hence the calculation of the magnitude of the 25 Hz small-amplitude magnetic field, which is proportional to the new Larmor frequency.

Figure 9 shows the magnetic field calculated from the measurement of the Larmor frequency after a 25 Hz 15 pT magnetic field was applied. A lowpass filter of a cutoff frequency of 50 Hz was used after the lock-in amplifier in order to remove the power line noise (at 50 Hz and its harmonics) as well as all high frequencies noise. It is obvious from Figure 9 that the small-signal 25 Hz magnetic field could be recovered (peak-to-peak magnitude is around 33 pT), demonstrating the capability of the optical Mx magnetometer to measure ultra-low-amplitude magnetic fields.

5. Conclusion

An optically pumped quantum magnetometer on Mx configuration has been developed and its capability to measure ultra-low-amplitude magnetic fields has been experimentally demonstrated. A high intrinsic sensitivity of 63 \(fT/Hz^{1/2}\) measured in a 1 Hz bandwidth has been achieved with an input optical power of 20 \(\mu\)W at a vapor cell temperature of 50°C. Experimental results have shown that the environmental noise can significantly drop the magnetometer sensitivity by several orders of magnitude to as low as 27 \(pT/Hz^{1/2}\). A high actual sensitivity of 21 \(pT/Hz^{1/2}\) has been attained with an input optical power of 20 \(\mu\)W at room temperature. The measured bandwidth of the magnetometer has been shown to vary between 100 Hz at room temperature and 25 Hz at 45°C. Experimental results have also shown that the ultimate best intrinsic sensitivity (327 \(fT/Hz^{1/2}\)) calculated over the measured bandwidth (26 Hz) can be attained with an input optical power of 20 \(\mu\)W at a vapor cell temperature of 48°C and that the environmental noise reduces this sensitivity to 130 \(pT/Hz^{1/2}\). Finally, the ability of the magnetometer to detect a 25 Hz sinusoidal magnetic field of amplitude as low as 15 pT has experimentally been demonstrated.

References


Research Article

Lyapunov Control of Quantum Systems with Impulsive Control Fields

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We investigate the Lyapunov control of finite-dimensional quantum systems with impulsive control fields, where the studied quantum systems are governed by the Schrödinger equation. By three different Lyapunov functions and the invariant principle of impulsive systems, we study the convergence of quantum systems with impulsive control fields and propose new results for the mentioned quantum systems in the form of sufficient conditions. Two numerical simulations are presented to illustrate the effectiveness of the proposed control method.

1. Introduction

In the last few years, because of a wide variety of applications of the quantum control theory, such as quantum chemistry, quantum information processing, and quantum electronics, considerable attention has been focused on quantum control theory, and the growing interest in this subject has been attributed to both theoretical and experimental breakthroughs ([1–9] and references therein); it indicates that quantum control has become an important area of research.

Controllability is one important part in the quantum control theory. Different definitions of controllability have been studied in [10–12], and sufficient conditions which are based on the Lie algebra of system Hamiltonian are also given. Referring to the control method, Lyapunov-based techniques are good approaches, such as implicit Lyapunov control [9, 13], Lyapunov functions based on state distance [5], average value of an imaginary mechanical quantity [14, 15], and state error [15, 16].

In [17], Turinici and Rabitz considered the wavefunction controllability method based on graph theory. When a quantum system is not wavefunction controllable with one control field, Dong and Petersen introduced the switching control method to drive the system by using two controllers to arbitrary target state based on graph theory [18]. In [19], Zhao et al. considered another switching control method of closed quantum systems, which was via the Lyapunov method.

Inspired by the switching control method, we developed the impulsive control method to drive a quantum system to a given target state. As we know, impulsive dynamical systems are a special class of dynamical systems, which exhibit continuous evolution typically described by ordinary differential equations and instantaneous state jumps or impulses. Nowadays, there has been increasing interest in the analysis and synthesis of impulsive systems, or impulsive control systems, due to their significance in both theory and applications; see [20–23] and the references therein.

By adding an impulsive control field besides the continuous control field, we apply the impulsive control method to control quantum systems. From the result in [24], when one control field contributes with given frequency, quantum systems governed by the Schrödinger equation can be described as impulsive dynamical systems.

In this paper, based on the Lyapunov method and invariant principle of impulsive systems [25], our attention is focused on the Lyapunov control of quantum systems with impulsive control fields. In Section 2, we present the quantum systems with impulsive control fields and introduce the invariant principle of impulsive systems. In Section 3, we give different control fields to drive quantum systems based on three Lyapunov functions and analyze the asymptotic stability of quantum systems with impulsive control fields. We justify the effectiveness of the proposed control fields in two simulation experiments in Section 4.
2. Notations and Definitions

Consider the impulsive dynamical system described by the following:

\[ \begin{align*}
\dot{x}(t) &= f_c(x(t)), \quad t \in (\tau_k, \tau_{k+1}), \\
\Delta x(t) &= f_d(x(t)), \quad t = \tau_k,
\end{align*} \]

where \( x(t) \in \mathbb{R}^n \) denotes the system state, \( f_c(x) \) is a continuous function from \( \mathbb{R}^n \) to \( \mathbb{R}^n \), the set \( E = \{ \tau_1, \tau_2, \ldots ; \tau_1 < \tau_2 < \cdots \} \subset \mathbb{R}^+ \) is an unbounded, closed, and discrete subset of \( \mathbb{R}^+ \) which denotes the set of times when jumps occur, and \( f_d : \mathbb{R}^n \to \mathbb{R}^n \) denotes the incremental change of the state at the time \( \tau_k \). In the \( n \)-dimensional complex space \( \mathbb{C}^n \), we choose the most common norm \( \|x\| := \sqrt{x^* x} \), where \( x \) is represented as a column vector \( (x_1, x_2, \ldots, x_n)^T \) and \( x^* \) denotes its conjugate transpose. Denote by \( M_n(\mathbb{C}) \) the space of \( n \times n \) complex matrices with an inner product \( (\cdot, \cdot) : M_n(\mathbb{C}) \times M_n(\mathbb{C}) \to \mathbb{C} \),

\[ (a, b) = \text{Tr}(ab), \]

and the norm \( \|a\|^2 = (a, a) \).

Consider the following \( n \)-level quantum system with two control fields, and set the Plank constant \( h = 1 \):

\[ i |\psi(t)\rangle = \left( \hat{H}_0 + f_1(t) \hat{H}_1 + \sum_{k=1}^{\infty} f_2(t) \hat{H}_2 \delta(t - \tau_k) \right) |\psi(t)\rangle, \]

where the ket \( |\psi(t)\rangle \in \mathbb{C}^n \) represents the state vector of quantum systems, which is right continuous, and the state vector evolves on or in a sphere with radius one, and we denote the set of quantum states by \( \mathcal{VS}_n \), and \( \delta(\cdot) \) is the Dirac impulse. Physically, two states \( |\psi_1\rangle \) and \( |\psi_2\rangle \) that differ by a phase \( \theta(t) \in \mathbb{R} \), that is, \( |\psi_1\rangle = \exp(i\theta(t)) |\psi_2\rangle \), describe the same physical state in or on the sphere \( \mathbb{S}^n \). We denote the bra associated with the ket \( |\psi(t)\rangle \) with \( \langle \psi(t)| \). When the quantum system evolves freely under its own internal dynamics, that is, there is no external field implemented on the system, just the free Hamiltonian \( \hat{H}_0 \) is introduced. \( \hat{H}_j \) (\( j = 1, 2 \)) represent the interaction energy between the system and the external classical control fields \( f_j(t) \) (\( j = 1, 2 \)) and are called interaction Hamiltonian. \( \hat{H}_j \) (\( j = 0, 1, 2 \)) are all \( n \times n \) self-adjoint operators in the \( n \)-dimensional Hilbert space \( \mathcal{H} \) and assumed to be time independent. In this paper, we set that the first control function \( f_1(t) \) is a continuous function, the other one \( f_2(t) \) only takes effect to quantum systems at the impulsive points \( E \).

Multiplying both sides of (3) by \( -i \), we have

\[ |\psi(t)\rangle = \left( \hat{H}_0 + f_1(t) \hat{H}_1 + \sum_{k=1}^{\infty} f_2(t) \hat{H}_2 \delta(t - \tau_k) \right) |\psi(t)\rangle, \]

where \( \hat{H}_j = -i \hat{H}_j \in M_n(\mathbb{C}) \) (\( j = 0, 1, 2 \)), skew-Hermitian matrices.

In quantum control, the target state is usually an eigenstate of the free Hamiltonian, and we set the target state \( |\psi_f\rangle \) satisfies:

\[ \hat{H}_0 |\psi_f\rangle = \lambda_f |\psi_f\rangle, \]

where \( \lambda_f \) is the eigenvalue of \( \hat{H}_0 \) corresponding to \( |\psi_f\rangle \).

By the same method in [24], we obtain that quantum systems (3) with impulsive control fields can be described as

\[ |\psi(t)\rangle = \left( \hat{H}_0 + f_1(t) \hat{H}_1 + \sum_{k=1}^{\infty} f_2(t) \hat{H}_2 \delta(t - \tau_k) + \omega I \right) |\psi(t)\rangle, \]

where \( I \) is the identity matrix. If the control field \( f_2(t) \) only takes effect at the impulsive points \( E \), the quantum systems with impulsive control fields are

\[ |\psi(t)\rangle = \left( \hat{H}_0 + f_1(t) \hat{H}_1 + \omega I \right) |\psi(t)\rangle, \quad t \neq \tau_k, \]

\[ \Delta |\psi\rangle = f_2(t) \hat{H}_2 |\psi(\tau_k)\rangle, \quad t = \tau_k. \]

Subject to quantum systems (3) or (7), we focus on finding control fields \( f_1(t) \) and \( f_2(\tau_k) \), such that the quantum systems with impulsive control field (6) or (8) are driven to target states. Firstly, we introduce the invariant principle of impulsive systems.

**Lemma 1** (see [25]). Consider the impulsive dynamical system (1), assume that \( \mathcal{D}_c \subset \mathcal{D} \) is a compact positively invariant set with respect to (1), and assume that there exists a \( C^1 \) function \( V : \mathcal{D}_c \to \mathbb{R} \) such that

\[ \begin{align*}
(1) \quad & V(x(t)) \leq 0, \quad x \in \mathcal{D}_c, \quad t \neq \tau_k; \\
(2) \quad & V(x(\tau_k)) + f_2(x(\tau_k)) \leq V(x(\tau_k)), \quad x \in \mathcal{D}_c, \quad t = \tau_k.
\end{align*} \]

Let \( G = \{ x \in \mathcal{D}_c : t \neq \tau_k, V(x(t)) = 0 \} \cup \{ x \in \mathcal{D}_c : t = \tau_k, V(x(\tau_k)) + f_2(x(\tau_k)) = V(x(\tau_k)) \} \), and let \( M \subset G \) denote the largest invariant set contained in \( G \). If \( x_0 \in \mathcal{D}_c \), then \( x(t) \to M \) as \( t \to \infty \).

3. Main Results

**Theorem 2.** For quantum system (6), if \( \hat{H}_0 \) is nondegenerate, set control fields \( f_1(t) = K_1g_1(\text{Im}(e^{i\langle \psi(t)|\psi\rangle}\langle \psi_f|\hat{H}_1|\psi(t)\rangle)) \)
and \( f_2(\tau_k) = K_2g_2(\text{Im}(e^{i\langle\psi(\tau_k)|\psi\rangle}\langle\psi_f|H_2|\psi(\tau_k))))) \) where constants \( K_1, K_2 > 0 \) and the image of function \( y_j = g_j(x_j) \) \((j = 1, 2)\) passes the origin of plane \( x_j-y_j \) monotonically and lies in quadrant I or III, then quantum systems with impulses (6) converge to the largest invariant set \( V_{S_n} \cap E_1 \) where \( E_1 = \{|\psi\rangle : \langle\psi|H_2|\psi\rangle = 0\}. \) If all the states in \( E_1 \) are equivalent to the target state \( |\psi\rangle \), then the systems will converge asymptotically to the target state \( |\psi_f\rangle \).

**Proof.** Choose the Lyapunov function based on the state distance

\[
V (|\psi (t)\rangle , t) = \frac{1}{2} \left( 1 - \left| \langle\psi_f|\psi (t)\rangle \right| \right)^2.
\]

When \( t \neq \tau_k \),

\[
\dot{V}_1 = - f_1 (t) \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \langle\psi (t)|\psi_f\rangle \right)
= - f_1 (t) \left| \langle\psi (t)|\psi_f\rangle \right| \text{Im} \left( e^{i\langle\psi (t)|\psi\rangle} \langle\psi_f|H_1|\psi (t)\rangle \right), \tag{9}
\]

as discussed in [15], by the control field

\[
f_1 (t) = K_1 g_1 \left( \text{Im} \left( e^{i\langle\psi (t)|\psi\rangle} \langle\psi_f|H_1|\psi (t)\rangle \right) \right), \tag{10}
\]

we have

\[
\dot{V}_1 (t) = - K_1 \left| \langle\psi (t)|\psi_f\rangle \right| \text{Im} \left( e^{i\langle\psi (t)|\psi\rangle} \langle\psi_f|H_1|\psi (t)\rangle \right)
\]

\[
\times g_1 \left( \text{Im} \left( e^{i\langle\psi (t)|\psi\rangle} \langle\psi_f|H_1|\psi (t)\rangle \right) \right) < 0 \quad (t \neq \tau_k). \tag{11}
\]

When \( t = \tau_k \),

\[
V (|\psi (\tau_k)\rangle , \tau_k) = V (|\psi (\tau_k^+)\rangle , \tau_k^+)
= \frac{1}{2} \left( 1 - \left| \langle\psi_f|H_2|\psi (\tau_k)\rangle \right| \right) 
\times \left( \langle\psi_f|H_2|\psi (\tau_k)\rangle \right)
\]

\[
= V (|\psi (\tau_k)\rangle , \tau_k) - f_2 (\tau_k) \langle\psi (\tau_k)|\psi_f\rangle \left| \langle\psi_f|H_2|\psi (\tau_k)\rangle \right| 
\times \text{Im} \left( e^{i\langle\psi (\tau_k)|\psi\rangle} \langle\psi_f|H_2|\psi (\tau_k)\rangle \right)
\]

\[
- \frac{1}{2} f_2 (\tau_k) \left| \langle\psi (\tau_k)|\psi_f\rangle \right| \left| \langle\psi_f|H_2|\psi (\tau_k)\rangle \right| \langle\psi_f|H_2|\psi (\tau_k)\rangle, \tag{12}
\]

by the control field

\[
f_2 (\tau_k) = K_2 g_2 \left( \text{Im} \left( e^{i\langle\psi (\tau_k)|\psi\rangle} \langle\psi_f|H_2|\psi (\tau_k)\rangle \right) \right), \tag{13}
\]

and \( \langle\psi (\tau_k)|\psi_f\rangle \langle\psi_f|H_2|\psi (\tau_k)\rangle > 0 \), we have

\[
V (|\psi (\tau_k)\rangle , \tau_k) < V (|\psi (\tau_k)\rangle , \tau_k), \tag{14}
\]

where \( K_j \) \((j = 1, 2)\) can be chosen properly to adjust the control amplitude. If \( \langle\psi (t)|\psi_f\rangle = 0 \), or \( \langle\psi (\tau_k)|\psi_f\rangle = 0 \), we set \( \mathcal{L} (\psi (t)|\psi_f) = 0 \), or \( \mathcal{L} (\psi (\tau_k)|\psi_f) = 0 \).

By the definition of invariant set and properties of limit point, if we choose the control field \( f_1 (t) \) (11) which is the same as that in [15], the largest invariant set of quantum systems with impulses (6) is \( V_{S_n} \cap E_1 \), where \( E_1 = \{|\psi\rangle : \langle\psi|H_2|\psi\rangle = 0\}. \) From the invariant principle Lemma 1, quantum systems with impulsive control fields (6) will converge to \( V_{S_n} \cap E_1 \).

Thus, we complete the proof. \( \square \)

When the phase \( \theta \) is considered, we choose the Lyapunov function based on the state error [15, 16].

**Theorem 3.** For quantum system (8), if \( H_0 \) is nondegenerate, set the control fields \( \lambda_f + \omega = K_0 g_0 \left( \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \right) \right), f_1 (t) = K_1 g_1 \left( \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \right) \right), \) and \( f_2 (\tau_k) = - 2 \text{Im} \left( \langle\psi (\tau_k)|\psi_f\rangle \right) / \sqrt{\text{Tr} (H_2^2)} \), where constants \( K_j > 0 \) \((j = 0, 1)\) and the image of function \( y_j = g_j(x_j) \) passes the origin of plane \( x_j-y_j \) monotonically and lies in quadrant I or III, then quantum systems with impulses (8) converge to the largest invariant set \( V_{S_n} \cap E_2 \), where \( E_2 = \{|\psi\rangle : \langle\psi|H_2|\psi\rangle = 0, \text{Im} \left( \langle\psi |H_2|\psi \rangle \right) = 0\}. \) If all the states in \( E_2 \) are equivalent to the target state \( |\psi_f\rangle \), then the systems will converge asymptotically to the target state \( |\psi_f\rangle \).

**Proof.** Choose the Lyapunov function based on the state error

\[
V (|\psi (t)\rangle , t) = \langle\psi (t) - \psi_f|\psi (t) - \psi_f\rangle. \tag{15}
\]

When \( t \neq \tau_k \),

\[
\dot{V} = - (\lambda_f + \omega) \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \right) 
- f_1 (t) \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \right), \tag{16}
\]

and the simple control field

\[
\lambda_f + \omega = K_0 g_0 \left( \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \right) \right), \tag{17}
\]

\[
f_1 = K_1 g_1 \left( \text{Im} \left( \langle\psi_f|H_1|\psi (t)\rangle \right) \right), \tag{18}
\]
we have
\[
\dot{V}(t) = -K_0 \Im \left( \langle \psi_f | \psi(t) \rangle \right) g_0 \left( \Im \left( \langle \psi_f | \psi(t) \rangle \right) \right) \\
- K_1 \Im \left( \langle \psi_f | \tilde{H}_1 \psi(t) \rangle \right) \\
\times g_1 \left( \Im \left( \langle \psi_f | \tilde{H}_1 \psi(t) \rangle \right) \right) < 0 \quad (t \neq \tau_k).
\]
When \( t = \tau_k \),
\[
V(\psi(\tau_k), \tau_k) = V(\psi(\tau_k^+), \tau_k^+)
\]
\[
= \left( \langle \psi(\tau_k^-) | (I - f_2(\tau_k) H_2) - \langle \psi_f \rangle \right) \\
\times \left( (I + f_2(\tau_k) H_2) \psi(\tau_k^-) \right) - \langle \psi_f \rangle \\
= \langle \psi(\tau_k^-) - \psi_f | \psi(\tau_k^-) - \psi_f \rangle \\
+ 2 f_2(\tau_k) \Im \left( \langle \psi(\tau_k^-) | \tilde{H}_2 \psi_f \rangle \right) \\
+ f_2^2(\tau_k) \langle \psi(\tau_k^-) | \tilde{H}_2^2 \psi(\tau_k^-) \rangle,
\]
\[
\text{since } \langle \psi(\tau_k^-) | \tilde{H}_2^2 \psi(\tau_k^-) \rangle \leq \| \psi(\tau_k^-) \|^2 \leq \sqrt{\Tr(H_2^2)}, \text{ by the control field } f_2(\tau_k) = -2 \Im(\langle \psi(\tau_k^-) | \tilde{H}_2 \psi_f \rangle) / \sqrt{\Tr(H_2^2)}.
\]
Using the control field \( \lambda_f + \omega_f, f_1(t) \) (18), the largest invariant set of quantum systems with impulsive control fields (8) is \( V S_n \cap E_2 \) [15, 16], where \( E_2 = \{ |\psi \rangle : \langle \psi_f | H_1 | \psi \rangle = 0, \Im(\langle \psi_f | \psi \rangle) = 0 \} \). From the invariant principle Lemma 1, the quantum systems with impulsive control fields (8) will converge to \( V S_n \cap E_2 \).

Thus, we complete the proof.

Set that the eigenvalues of \( H_0 \) are \( \lambda_j, j \in \{1, 2, \ldots, n\} \), and the corresponding eigenstates are \( |\phi_j \rangle, j \in \{1, 2, \ldots, n\} \).

**Theorem 4.** For quantum systems with impulsive control field (6), if \( H_0 \) is nondegenerate, set \( f_1(t) = -K_1 \langle \psi(t) | i\tilde{H}_1 Q | \psi(t) \rangle \), and \( f_2(\tau_k) = -\langle \psi(\tau_k^-) | i\tilde{H}_2 Q | \psi(\tau_k^-) \rangle / \sqrt{\Tr(Q\tilde{H}_1^2)} \), where constant \( K_1 > 0 \), \( Q \) is a positive definite Hermitian matrix and satisfies \( |H_0, Q| = 0 \), then quantum systems with impulsive control field (6) converge to the largest invariant set \( V S_n \cap E_3 \), where \( E_3 = \{ |\psi \rangle : \langle \phi_j | H_1 | \phi_k \rangle \langle \phi_k | \psi \rangle \langle \psi | \phi_j \rangle = 0, j, k \in \{1, 2, \ldots, n\} \} \). From the invariant principle Lemma 1, the quantum systems controlled by \( f_1(t), f_2(\tau_k) \) (6) will converge to \( V S_n \cap E_3 \).

Thus, we complete the proof.

**Proof.** Choose another Lyapunov function based on the average value of an imaginary mechanical quantity
\[
V (|\psi(t)\rangle, t) = \langle \psi(t) | Q | \psi(t) \rangle.
\]
Considering the case \( t \neq \tau_k \), one has
\[
\dot{V}(t) = \langle \psi(t) | [i\tilde{H}_0, Q] | \psi(t) \rangle \]
\[
+ f_1(t) \langle \psi(t) | i\tilde{H}_1 Q | \psi(t) \rangle,
\]
and since there is no relation between \( [i\tilde{H}_0, Q] \) and the control component, we can set \( [i\tilde{H}_0, Q] \) for convenience. If we choose simple and effective control field
\[
f_1(t) = -K_1 \langle \psi(t) | i\tilde{H}_1 Q | \psi(t) \rangle,
\]
where \( K_1 > 0 \), then \( \dot{V}(t) = -K_1 \langle \psi(t) | i\tilde{H}_1 Q | \psi(t) \rangle^2 < 0 \).

Since the state \( |\psi(t)\rangle \) is right continuous at the impulsive points, we have
\[
V (|\psi(\tau_k)\rangle, \tau_k)
\]
\[
= V (|\psi(\tau_k^-)\rangle, \tau_k^-)
\]
\[
= \langle \psi(\tau_k^-) | (I - f_2(\tau_k) H_2) - \langle \psi_f \rangle \right) \\
\times \left( (I + f_2(\tau_k) H_2) \psi(\tau_k^-) \right) - \langle \psi_f \rangle \\
= \langle \psi(\tau_k^-) - \psi_f | \psi(\tau_k^-) - \psi_f \rangle \\
+ 2 f_2(\tau_k) \Im \left( \langle \psi(\tau_k^-) | \tilde{H}_2 \psi_f \rangle \right) \\
+ f_2^2(\tau_k) \langle \psi(\tau_k^-) | \tilde{H}_2^2 \psi(\tau_k^-) \rangle
\]
\[
\leq V (|\psi(\tau_k^-)\rangle, \tau_k^-).
\]

For Hermitian matrices \( Q \) and \( \tilde{H}_2, \langle \psi(\tau_k^-) | i\tilde{H}_2 Q | \psi(\tau_k^-) \rangle \) and \( \langle \psi(\tau_k^-) | i\tilde{H}_2 Q \tilde{H}_2 | \psi(\tau_k^-) \rangle \) are real numbers, and
\[
\langle \psi(\tau_k^-) | i\tilde{H}_2 Q \tilde{H}_2 | \psi(\tau_k^-) \rangle \leq \| \psi(\tau_k^-) \|^2 \| \tilde{H}_2 Q \tilde{H}_2 \|
\]
\[
\leq \sqrt{\Tr(Q\tilde{H}_2^2)}.
\]

By the control function \( f_2(\tau_k) = -\langle \psi(\tau_k^-) | i\tilde{H}_2 Q | \psi(\tau_k^-) \rangle / \sqrt{\Tr(Q\tilde{H}_2^2)} \), we have
\[
V (|\psi(\tau_k^-)\rangle, \tau_k^-) < V (|\psi(\tau_k^-)\rangle, \tau_k^-).
\]

Using the control field \( f_1(t) \) (24), the largest invariant set of quantum systems with impulsive control field (6) is \( V S_n \cap E_3 \) [15], where \( E_3 = \{ |\psi \rangle : \langle \phi_j | H_1 | \phi_k \rangle \langle \phi_k | \psi \rangle \langle \psi | \phi_j \rangle = 0, j, k \in \{1, 2, \ldots, n\} \} \). From the invariant principle Lemma 1, the quantum systems controlled by \( f_1(t), f_2(\tau_k) \) (6) will converge to \( V S_n \cap E_3 \).

Thus, we complete the proof.
4. Illustrative Examples

In this section, in order to illustrate the effectiveness of the proposed method in this paper, two numerical simulations have been presented for two five-level quantum systems and the fourth-order Runge-Kutta method is used to solve with time steps size 0.06.

**Example 1.** Consider the five-level quantum system with internal Hamiltonian, the first control Hamiltonian \[\tilde{H}_0\] and the second control Hamiltonian given as follows:

\[
\tilde{H}_0 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1.2 & 0 & 0 & 0 \\
0 & 0 & 1.3 & 0 & 0 \\
0 & 0 & 0 & 2 & 0 \\
0 & 0 & 0 & 0 & 2.15
\end{pmatrix},
\]

\[
\tilde{H}_1 = \begin{pmatrix}
0 & 0 & 1 & 1 & 0 \\
1 & 0 & 0 & 1 & 1 \\
1 & 0 & 0 & 1 & 1 \\
1 & 1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0
\end{pmatrix},
\]

\[
\tilde{H}_2 = \begin{pmatrix}
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 \\
0 & 0 & 1 & 0 & 1 \\
1 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 1 & 0
\end{pmatrix}.
\]

Let the initial state and the target state be \(|\psi_0\rangle = (1 \ 0 \ 0 \ 0 \ 0)^T\) and \(|\psi_f\rangle = (0 \ 0 \ 0 \ 0 \ 1)^T\), respectively. The parameters are chosen as \(K_1 = 0.15, K_2 = 0.001\). Setting the state \(|\psi(t)\rangle = (x_1 \ x_2 \ x_3 \ x_4 \ x_5)^T\), by the control fields

\[
f_1(t) = K_1 \text{Im}(e^{i\langle\psi(t)|\psi(t)\rangle} \langle \psi_f | H_1 | \psi(t) \rangle),
\]

\[
f_2(\tau_k) = K_2 \text{Im}(e^{i\langle\psi(\tau_k)|\psi\rangle} \langle \psi_f | H_2 | \psi(\tau_k) \rangle),
\]

we have the simulation result shown in Figure 1. It demonstrates the control performance with impulsive control field \(f_2(\tau_k)\), and the final transition probability attains about 0.94149, which excels the one (about 0.93785) in [15].

**Example 2.** Consider the five-level quantum system with internal Hamiltonian and the control Hamiltonians given as follows:

\[
\tilde{H}_0 = \begin{pmatrix}
1 & 0 & 0 & 0 & 0 \\
0 & 1.1 & 0 & 0 & 0 \\
0 & 0 & 1.2 & 0 & 0 \\
0 & 0 & 0 & 1.4 & 0 \\
0 & 0 & 0 & 0 & 1.7
\end{pmatrix},
\]

\[
\tilde{H}_1 = \begin{pmatrix}
0 & 0 & 0 & 1 & 1 \\
0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 1
\end{pmatrix},
\]

\[
\tilde{H}_2 = \begin{pmatrix}
0 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 \\
1 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 1 \\
0 & 1 & 0 & 1 & 0
\end{pmatrix}.
\]

Let the initial state and the target state also be \(|\psi_0\rangle = (1 \ 0 \ 0 \ 0 \ 0)^T\) and \(|\psi_f\rangle = (0 \ 0 \ 0 \ 0 \ 1)^T\), respectively. The parameters are chosen as \(K_1 = 0.15, K_2 = 0.001\). Setting the state \(|\psi(t)\rangle = (x_1 \ x_2 \ x_3 \ x_4 \ x_5)^T\), by the same control fields in Example 1, we have the simulation results shown in Figure 2. In Figure 2(a), the population of the system with impulsive control field \(f_2(\tau_k)\) is shown, and the result shown in Figure 2(b) demonstrates the control performance without impulsive control field. The quantum system whose Hamiltonians are (30) is driven to the target state \(|\psi_f\rangle\), and the final transition probability attains about 0.99942 in Figure 2(a), which is better than the one (about 0.99581) in Figure 2(b), and significantly, the control method with one impulsive control field can prevent the evolution from decaying.

5. Conclusion

In this paper, we have introduced the Lyapunov control method to quantum systems with impulsive control fields and...
given three kinds of control fields based on different Lyapunov functions. The theoretical results have been verified by numerical simulations to illustrate the effectiveness and advantages of the proposed method compared with existing results.

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References


