1 Introduction

The theory of quantum mechanics was one of the major discoveries of the history of science in the twentieth century. It is very important to study the properties of quantum mechanical systems and their control. As quantum technologies have matured, a lot of practical applications of quantum control have been realized in quantum optics, cavity quantum electro-dynamics (OED), atomic spin ensembles, ion trapping, and Bose-Einstein condensation, and so on, which means that the manipulation of quantum phenomena is a rapidly growing research field. The improvements in nanotechnology and its manufacture process as well as increasing interests in new applications of quantum effects, including quantum information process, mean the control of quantum phenomena is becoming a growing concern all over the world in areas such as quantum computation, quantum chemistry, nano-material, and quantum physics. In the past three decades, researchers have been trying to expand the control theories that are obtained from the macroscopic world to the microscopic world, and this has gradually become a new system control theory in interdisciplinary fields: quantum control theory. The methods and technologies of quantum control have become one of the leading research areas in the world. The main topics of quantum control theory are, from the control system perspective, to investigate how to manipulate a system state trajectory and its evolution. For this purpose, quantum control theory is used to design an external realizable control law to achieve a desired control goal by combining control theory and the characteristics of quantum systems. Developing a special control theory and methods for quantum systems has been a challenging task. This task requires interdisciplinary researchers with interest in the development and applications of novel quantum control methodologies to fundamental physical, chemical, and biological problems from the quantum physics, chemistry, quantum information, mathematical and computer sciences, and control engineering communities. On the other hand, the field of quantum information involves the complex task of designing and effectively manipulating multi-qubit systems. However, this problem is beset by significant difficulties, such as the corruption of quantum information caused by decoherence. Finding solutions to the problem of decoherence, resulting from the unavoidable interaction of a quantum system with its environment, is one of the most critical challenges impeding practical realization of a quantum information processor (QIP). Current strategies for decoherence management are being developed by researchers from three distinct communities within quantum information science (QIS), namely, dynamical decoupling (DD), optimal control (OC), and quantum error correction (QEC). All of the

problems to be solved in these areas are in fact control problems, which should be solved by means of control theory and methods. The aim of a control theory is to find a method of transforming a system by means of controlling action in order to achieve its prescribed behavior. A control theory can be used effectively only when it is executed in the whole process of control systems design because control theory is one part of the whole process of control systems design.

The whole process of control system design and implementation, which can also be called control system engineering, in the order in which it is done is (i) modeling, including identification, estimation, and filter; (ii) system synthesis, including controllability, observability, and/or reachability; (iii) control laws design; (iv) control systems analysis, including stability and/or convergence; (v) the numerical simulation of the control system; and (vi) actual system experimental implementation. A designer could do every part of the process if necessary, but because it is a huge control engineering process in fact it is better for one person to study only one or two parts of the design. The problems that exist in each part of the process may be solved by several available theories, methods, or tools, so in practice no one person can do all the control system design and implementation. In most cases the focus is on the study of control methods for a system in which the model of a system to be controlled does not need to be built because it is given. The controllability does not be studied because it is known that the system to be controlled is controllable. If it is not the case, controllability analysis has to be done. No-one can design a control law for an uncontrollable system. In other words, no control method can be used to achieve the desired behavior for an uncontrollable system. Not doing some work in a control system design does not mean that it is not important, but that it is known or the requirement has been satisfied. This book is mainly concerned with steps (iii) to (v) of the process of control system design. Because the quantum control system concerns interdisciplinary knowledge, let us start with quantum states.

1.1 Quantum States

A quantum system can be completely described by its state vector $|\psi\rangle$ in a complex vector space with an inner product known as Hilbert space. $|\psi\rangle$ is a unit vector in the system's state space and is called the wave function. In physics, bra-ket notation is often used to denote such vectors. The notation $|\bullet\rangle$ is represented by a single vector known as a ket, while $\langle \bullet |$ is a bra. This notation is known as Dirac representation in a complex Hilbert space *H*. A quantum state is also called as a qubit. The wave function $|\psi\rangle$ represents a pure state. This "state" in quantum mechanics is different from that in classical systems. For a classical system, the state usually describes some real physical properties such as the position or the momentum, which are generally observable. However, a quantum state $|\psi\rangle$ cannot be directly observed and also does not directly correspond to the physical quantity of the quantum system. Since the global phase of a quantum state $|\psi\rangle$ has no observable physical effect, we often say that the vectors $|\psi\rangle$ and $e^{i\alpha}|\psi\rangle$, in which $i = \sqrt{-1}$ and $\alpha \in \mathbb{R}$, describe the same physical state. For example, in quantum information theory the information is coded by a two-level (two-state) quantum system and the state $|\psi\rangle$ of a qubit can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\alpha}\sin\frac{\theta}{2}|1\rangle$$
(1.1)

where $\theta \in [0, \pi]$ and $\alpha \in [0, 2\pi]$. Then $|0\rangle$ and $|1\rangle$ correspond to the states 0 and 1 for a classical bit.

A quantum system can be closed or open according to whether or not the system is isolated from the external environment. The closed quantum system is under conditions of absolute zero temperature or does not interact with the external environment, and its state evolution is unitary. However, quantum systems usually cannot meet these ideal conditions in practical quantum information processing and quantum computing, and have interactions with the external environment, and are therefore treated as open quantum systems. In practical applications, the quantum systems to be controlled are usually not simple closed systems. They may be quantum ensembles or open quantum systems and their states cannot be written in the form of unit vectors $|\psi\rangle$. In this case, it is necessary to introduce the density operator or density matrix $\rho : H \to H$ to describe quantum states of quantum ensembles or open quantum systems. A density operator ρ is positive and has a trace equal to one. Suppose that a quantum system is in an ensemble $\{p_j, |\psi_j\rangle\}$ of pure states; that is, in a mixture of a number of pure states $|\psi_i\rangle$ with respective probabilities p_i . The density matrix for the system is defined as

$$\rho = \sum_{j} p_{j} |\psi_{j}\rangle \langle\psi_{j}| \tag{1.2}$$

where $\langle \psi_j | = (|\psi_j\rangle)^{\dagger}$ and $\sum_j p_j = 1$. Here, the operation (•)[†] refers to the conjugate transpose.

For a pure state $|\psi\rangle$, there is $\rho = |\psi\rangle\langle\psi|$ and $tr(\rho^2) = 1$. If the state ρ of a quantum system satisfies $tr(\rho^2) < 1$, we call the quantum state a mixed state.

A composite quantum system assumed to be made up of two subsystems *A* and *B* is defined on a Hilbert space $H = H_A \otimes H_B$, which is the tensor product of the Hilbert spaces H_A and H_B . For the composite quantum system, its state ρ_{AB} can be described by the tensor product of the states of its subsystems: $\rho_{AB} = \rho_A \otimes \rho_B$. Consider any bipartite pure state $|\psi\rangle_{AB}$. If it can be written as a tensor product of pure states $|\varphi\rangle_A \in H_A$ and $|\vartheta\rangle_B \in H_B$,

$$|\psi\rangle_{AB} = |\varphi\rangle_A \otimes |\vartheta\rangle_B \tag{1.3}$$

we call it a separable state; otherwise, we call it an entangled state. Quantum entanglement is a uniquely quantum mechanical phenomenon that plays a key role in many interesting applications of quantum communication and quantum computation.

When performing a particular measurement on a quantum state, the result is usually described by a probability distribution, and the distribution is completely determined by the quantum state and the observable describing the measurement. These probability distributions are necessary for both mixed states and pure states.

1.2 Quantum Systems Control Models

There are some different descriptions of a system model to be controlled. If the system to be controlled is a closed quantum system, its model is generally described by the Schrödinger or quantum Liouville equations, both of which are bilinear models. Bilinear models are widely used to describe closed quantum control systems such as molecular systems in physical chemistry and spin systems in nuclear magnetic resonance (NMR). For example, consider a spin-1/2 system in a constant magnetic field along the *z*-axis and controlled by magnetic fields along the *x*-axis and *y*-axis.

1.2.1 Schrödinger Equation

The Schrödinger equation, describing states of quantum particles, has analytical solutions that determine precisely how the state changes with time. The state $|\psi(t)\rangle$ of a closed quantum system evolves according to the Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}|\psi(t)\rangle = H_0|\psi(t)\rangle, |\psi(t=0)\rangle = |\psi_0\rangle$$
(1.4)

where H_0 is the free Hamiltonian of the system and a Hermitian operator on H, and \hbar is the reduced Planck's constant. For convenience, we usually assume $\hbar = 1$. For simplicity, we consider finite dimensional quantum systems, which are appropriate approximations in many practical situations.

The control of the system may be realized by a set of control functions $u_k(t) \in \mathbb{R}$ coupled to the system via time-independent interaction Hamiltonians $H_k(k = 1, 2, ...)$. Then the total Hamiltonian $H(t) = H_0 + \sum_{k} u_k(t)H_k$ determines the controlled evolution

$$i\frac{\partial}{\partial t}|\psi(t)\rangle = \left(H_0 + \sum_k u_k(t)H_k\right)|\psi(t)\rangle \tag{1.5}$$

Equation 1.5 is a bilinear quantum system control model.

1.2.2 Liouville Equation

If we use the density matrix $\rho(t)$ to describe the state of a closed quantum system, the evolution equation of the density matrix $\rho(t)$ can be described by the quantum Liouville equation

$$i\dot{\rho}(t) = [H(t), \rho(t)] \tag{1.6}$$

where $[H, \rho] = H\rho - \rho H$ is the commutation operator.

A control system with density matrix $\rho(t)$ as its state has the control system model

$$i\frac{\partial}{\partial t}\rho(t) = \left[H_0 + \sum_k u_k(t)H_k, \rho(t)\right]$$
(1.7)

where $\rho(t)$ is the variable to be controlled, H_0 is the free (or internal) Hamiltonian, and H_k is the control (or external) Hamiltonian. Usually we can assume that H_0 and H_k are all independent of time; $u_k(t)$ is an external control field, which is a real value.

Generally, the evolution of a Hamiltonian system is unitary in a closed quantum system. Unitary evolution preserves the spectrum of the quantum state, that is, the eigenvalues of the density matrix. All density matrices that have the same eigenvalues form a set of unitarily equivalent states, for example the set of all pure states. The control problem involving pure states is always expected to be described by the wave function $|\psi\rangle$ and its Schrödinger equation in Hilbert space. Equation 1.7 can also be used to control a mixed state. In practice, the system equation chosen depends on the problem to be solved. Compared to the Liouville equation, the Schrödinger equation in which the wave function is a variable is simple. However, the wave function can be used only in the pure states systems and not in the systems of mixed

states. There is no such a limitation for the Liouville equation with density matrix $\rho(t)$ as its variable. When pure states are manipulated, Equation 1.5 is equivalent to the expression of density operator as $\rho(t) = |\psi\rangle\langle\psi|$. But Equation 1.7 is valid for mixed states manipulations. It is to be noted that although we can regard the model in Equation 1.5 as a particular case of Equation 1.7, the case in Equation 1.5 for pure states always gives more straightforward results and provides some inspiring ideas for studying Equation 1.7.

1.2.3 Markovian Master Equations

In many practical applications, the quantum systems to be controlled are open quantum systems. In fact, this is the case for most quantum control systems since such systems unavoidably interact with their external environments, including control inputs and measurement devices. For an open quantum system, a quantum master equation with the density matrix $\rho(t)$ is suitable for describing the characteristics of the state. One of the simplest cases is when a Markovian approximation can be applied where a short environmental correlation time is supposed and memory effects may be neglected. For an *N*-dimensional open quantum system with Markovian dynamics, the state $\rho(t)$ can be described by the following Markovian master equation:

$$\dot{\rho}(t) = -\frac{i}{\hbar}[H,\rho] + \mathcal{L}\rho \tag{1.8}$$

where the generator \mathcal{L} of the semigroup represents a super-operator. The explicit form of this matrix can be derived using rigorous master equation formalism. The first term of Equation 1.8 describes the standard dynamics and the last term accounts for the gain and the damping mechanism, which has the form of the Liouville super-operator and can be written in the Lindblad form (Dacies, 1976):

$$\mathcal{L}\rho = \sum \left[F_i^{\dagger} F_i \rho + \rho F_i^{\dagger} F_i - 2F_i \rho F_i^{\dagger} \right]$$
(1.9)

where F_i and F_i^{\dagger} form a collection of generalized atomic creation and annihilation operators characteristic for a particular problem.

The Lindblad form of the master equation guarantees that the interaction with the damping reservoir preserves the positivity of the density operator.

1.2.4 Non-Markovian Master Equations

In the case of weak coupling, assuming the form of the interaction Hamiltonians between the system and the environment is bilinear, the two-level reduced system model described by the non-Markovian time-convolution-less master equation can be written as follows:

$$\dot{\rho}_s = -\frac{i}{\hbar} [H, \rho_s] + \mathcal{L}_t(\rho_s) \tag{1.10}$$

$$\mathcal{L}_{t}(\rho_{s}) = \frac{\Delta(t) + \gamma(t)}{2} \left(\left[\sigma_{-}\rho_{s}, \sigma_{-}^{\dagger} \right] + \left[\sigma_{-}, \rho_{s}\sigma_{-}^{\dagger} \right] \right) + \frac{\Delta(t) - \gamma(t)}{2} \left(\left[\sigma_{+}\rho_{s}, \sigma_{+}^{\dagger} \right] + \left[\sigma_{+}, \rho_{s}\sigma_{+}^{\dagger} \right] \right)$$
(1.11)

where $H = H_0 + \sum_k u_k(t)H_k$ is the total Hamiltonian, $H_0 = \frac{1}{2}\omega_0\sigma_z$ and H_m are the system and control Hamiltonian, respectively, ω_0 is the transition frequency of the two-level system, and

 $f_m(t)$ is the modulation by the time-dependent external control field. The control Hamiltonians can be described by $H_m = \sigma_i$ (i = x, y, z), where σ_x , σ_y , σ_z are the Pauli matrices σ and $\sigma_{\pm} = \frac{\sigma_x \pm i\sigma_y}{2}$ are the rising and lowering operators, respectively. $\mathcal{L}_t(\rho_s)$ describes the interaction between the system and the environment. In the Ohmic environment, the analytic expression for the dissipation coefficient $\gamma(t)$ appearing in Equation 1.11 is

$$\gamma(t) = \frac{\alpha^2 \omega_0 r^2}{1 + r^2} \{ 1 - e^{-r\omega_0 t} [\cos(\omega_0 t) + r\sin(\omega_0 t)] \}$$
(1.12)

and the diffusion coefficient $\Delta(t)$ is (Maniscalco *et al.*, 2004):

$$\Delta(t) = \alpha^2 \omega_0 \frac{r^2}{1+r^2} \{ \coth(\pi r_0) - \cot(\pi r_c) e^{-\omega_c t} [r \cos(\omega_0 t) - \sin(\omega_0 t)] \\ + \frac{1}{\pi r_0} \cos(\omega_0 t) [\overline{F}(-r_c, t) + \overline{F}(r_c, t) - \overline{F}(ir_0, t) - \overline{F}(-ir_0, t)] \\ - \frac{1}{\pi} \sin(\omega_0 t) [\frac{e^{-v_1 t}}{2r_0(1+r_0^2)} [(r_0 - i)\overline{G}(-r_0, t) + (r_0 + i)\overline{G}(r_0, t)] \\ + \frac{1}{2r_c} [\overline{F}(-r_c, t) - \overline{F}(r_c, t)] \}$$
(1.13)

where α is the coupling constant, $r_0 = \omega_0/2\pi kT$, $r_c = \omega_c/2\pi kT$, $r = \omega_c/\omega_0$ (kT is the environment temperature), ω_c is the high-frequency cutoff, $\overline{F}(x,t) \equiv {}_2F_1(x, 1, 1 + x, e^{-\nu_1 t})$, $\overline{G}(x,t) \equiv {}_2F_1(2, 1 + x, 2 + x, e^{-\nu_1 t})$ and ${}_2F_1(a, b, c, z)$ is the Gauss hypergeometric function (Gradshtein and Ryzhik, 1994).

Under conditions of high temperature, one has

$$\Delta(t)^{HT} = 2\alpha^2 kT \frac{r^2}{1+r^2} \left\{ 1 - e^{-r\omega_0 t} \left[\cos(\omega_0 t) - \frac{1}{r} \sin(\omega_0 t) \right] \right\}$$
(1.14)

From Equations 1.12 and 1.14, at high temperature both $\gamma(t) \approx 0$ and $|\Delta(t)| \gg \gamma(t)$ hold. In such a case, the diffusion coefficient $\Delta(t)$ plays a dominant role in the non-unitary dynamics of the system. The essential difference between Markovian systems and non-Markovian systems is the existence of the environment memory effect. If the decay rate is defined as $\beta_{1,2}(t) = \frac{\Delta(t) \pm \gamma(t)}{2}$, then the difference is distinguished by the sign of $\beta_i(t)$, that is, when $\beta_i(t) \ge 0$, the system mainly presents Markovian characteristics; when $\beta_i(t) < 0$, non-Markovian characteristics are predominant. In the case of high temperature, one can easily get $\beta_1(t) \approx \beta_2(t) = \frac{\Delta(t)}{2} = \beta(t)$ since $\gamma(t) \approx 0$. Note that at medium and low temperatures the approximation conditions in the Gauss hypergeometric function used to derive Equation 1.14 are not available, and $\gamma(t)$ can no longer be negligible, so $\beta_i(t)$ is related to both $\Delta(t)$ and $\gamma(t)$.

1.3 Structures of Quantum Control Systems

Systems, in one sense, are devices that take input and produce an output. A system can be thought to operate on the input to produce the output. The output is related to the input by a

relationship known as the system response. The system response usually can be modeled by a mathematical relationship between the system input and the system output. A control system is a device, or a set of devices, that manages, commands, directs, or regulates the behavior of other devices or systems.

Control systems are broadly classified as either closed-loop or open-loop control systems. From the system control point of view, whether or not a system is feedback (or closed-loop) control depends on the expression of its control law: it is feedback when control law is a function of the output variable of the system. An open-loop control system is controlled directly and runs only in pre-arranged ways, or only by an input signal. Open-loop control systems do not make use of feedback. The benefit of an open-loop system is often the low cost associated with running the processes. In this case, there is no need for feedback to be taken into consideration. The drawbacks of the open-loop system are less accuracy of control and less robustness of the disturbance and uncertainty because no measurement of the system output is used to alter the control. The open-loop control has been very successful in the control of some simple quantum systems. However, it has had some difficulties in more complex quantum control tasks such as suppressing the decoherence and dealing with the disturbances in quantum systems. A natural solution to this problem is to explore closed-loop control strategies.

In closed-loop control the system is self-adjusting. Data do not flow one way. They may pass back from a specific device to the start of the control system, telling it to adjust itself accordingly. Feedback loops take the system output into consideration, which enables the system to adjust its performance to meet a desired output response. Figure 1.1 is a basic feedback control system structure in which the output value of the system *y* is used to help prepare the next output value. In this way, one can create a system that correct error *e*. Figure 1.1 shows a feedback loop with the value 1. We call this a unity feedback control system.

A feedback control has many advantages: (i) it can increase the robustness of the system; (ii) it can increase the stability of the control system; (iii) it can automatically implement the control; and (iv) it can increase the performance of a control system. It is not an exaggeration to say that the outstanding achievements of control theory in engineering, including aeronautics and astronautics, in the last 50 years have become possible owing to the development of efficient feedback design methods.

As we know, feedback is an effective strategy in classical control theory and the aim of feedback is to compensate for the effects of unpredictable disturbances on a system under control or to make automatic control possible when the initial state of the system is unknown. In classical control, many results have shown that feedback control is superior to open-loop control. In feedback control, it is usually necessary to obtain information about the state of the system through measurement. However, the measurements of a quantum system will unavoidably destroy the state of the measured quantum system, which makes the situation more complex



Figure 1.1 Basic feedback control system structure

when applying feedback to quantum systems. In spite of this difficulty, important progress has been made and feedback has been used to improve the control performance for squeezed states (Chen and Elliott, 1990; Misawa and Kobayashi, 2000), quantum entanglement (Malk-mus *et al.*, 2005), and quantum state reduction (Muller *et al.*, 1990; Assion *et al.*, 1996) in many areas such as quantum optics (Herek, Materny, and Zewail, 1994), superconducting quantum systems (Assion *et al.*, 1996), Bose–Einstein condensate (Cerullo *et al.*, 1996), and nanomechanical systems (Bardeen *et al.*, 1998).

In quantum feedback control, the two main approaches to information acquisition are projective measurement and continuous weak measurement. The system to be controlled is a quantum system. However, the controller may be quantum, classical, or a quantum/classical hybrid. Several paradigms of quantum feedback have been proposed, such as Markovian quantum feedback (Brixner, Damrauer, and Gerber, 2001), Bayesian quantum feedback (Dupont et al., 1995), and coherent quantum feedback (Brown and Rabitz, 2002). In Markovian quantum feedback, any time delay is ignored and a memory-less controller is assumed, that is, the measurement record is immediately fed back into the system to alter the system dynamics and may then be forgotten (Knutsen et al., 2004). Hence, the equation describing the resulting evolution is a Markovian master equation. In Bayesian quantum feedback, the process is divided into two steps involving state estimation and feedback control. The best estimates of the dynamical variables are obtained continuously from the measurement record and feed back to control the system dynamics (Dupont et al., 1995). In coherent quantum feedback, the feedback controller itself is a quantum system and it processes quantum information. Feedback control is typically a closed-loop control system. In fact, a feedback control system with the output state obtained from mathematical models can also be designed. The premise of state feedback based on mathematical models is that the state of the system rightly evolves according to the mathematical model, which requires a closed quantum system due to the requirement of consistency between states from the model and from the real system.

1.4 Control Tasks and Objectives

In contrast to the states controlled in macroscopic systems, the states in quantum systems and their applications involve the manipulation and tracking of some particular states, such as active control in the molecular dynamics of the chemical reaction to selectively obtain the resultant, using the laser intensity and phase to manipulate the system's population, which transfers the molecular system from a initial base state to an excited state with high probability. In quantum computation, population transfer to the target state by radiation-induced excitation of atoms and molecules is in fact a kind of computing operation, and population transfer is used to prepare initial pure states. Fast parallel computing in a quantum system depends on its particular coherence, which is the computation of the superposition states. In quantum application of secret communication, the most important quantum states used are entangled states. The preparation, manipulation, and preservation of quantum states are the aims of using quantum control methods.

Generally, the objective in a control system, according to Figure 1.1, is to make some output, say y, behave in a desired way by manipulating some input, say u. The simplest objective might be to keep y small (or close to some equilibrium point), a regulation or manipulation problem, or to keep y - r small for r, a reference or command signal, in some set, the trajectory tracking

problem. From the control system perspective, the control tasks and objectives of a quantum system can be itemized as follows:

- 1. The state preparation: to obtain the prescribed state from the arbitrary initial state.
- 2. The state-to-state transition: to transfer a given initial state to a desired target state. The state-to-state transition is also called state-transition control. There is also a special state-transition control called population transfer control or population control. The control goal of this type of control task is to drive a quantum system from an initial given state (or population) to a pre-determined target state (or population).
- 3. The gate control and evolution control.
- 4. The trajectory tracking: to track the trajectory of a reference system.
- 5. The state preservation: to maintain the state unchanged.

The first four tasks can be for both closed and open quantum systems, while the fifth is the control goal specifically for open quantum systems.

1.5 System Characteristics Analyses

1.5.1 Controllability

Controllability is a major issue in system analysis before a control strategy is applied, and is used to judge whether it is possible to control or stabilize the system. The controllability relates to the possibility of controlling a particular system by using an appropriate control signal. If the system is not controllable, then no control signal will be able to manipulate its state. The controllability of quantum systems is a fundamental theoretical notion in quantum control as well as having practical importance because of its close connection with the universality of quantum computation and the possibility of attaining atomic- or molecular-scale transformations. We can more precisely define the concept of controllability: A state x_0 is controllable at time t_0 if for some finite time t_1 there exists an input u(t) that transfers the state x(t) from x_0 to the origin at time t_1 . In this book, we assume that the systems to be controlled are all controllable.

Generally, the results on the controllability of quantum systems only show if the system is controllable, but do not provide constructive methods to design a control law for manipulating a quantum system from an initial state to a predetermined target state. If a quantum system is controllable, the design of a proper control law to realize desired control goals is another important task, and one that this book will consider. Hence, it is desirable to develop useful methods to design such a control law, and these will be provided in this book.

1.5.2 Reachability

The reachability is also an important essential characteristic of a system. We can write the definition of reachability more precisely: A state x_1 is called reachable at time t_1 if for some finite initial time t_0 there exists an input u(t) that transfers the state x(t) from the origin at t_0 to x_1 . A system is reachable at time t_1 if every state x_1 in the state space is reachable at time t_1 . Similar to the controllability, if a system is reachable then one can design a control law to manipulate its state to reach the target state.

The difference between the controllability and the reachability is that the former refers to the possibility of transferring a system state to the origin, while the latter refers to the possibility of transferring a system state from an initial state to the target state. So in a quantum control system, the controllability in fact refers to the reachability.

1.5.3 Observability

The term observability describes whether or not the internal state variables of the system can be externally measured. If a state is not observable, the controller will not be able to determine the behavior of an unobservable state and hence cannot use it to stabilize the system directly. If a system is said to be observable at time t_0 with the system in state $x(t_0)$, it is possible to determine this state from the observation of the output over a finite time interval.

Controllability (reachability) and observability play an important role in the design of control systems in state space. In fact, the conditions of controllability and observability may govern the existence of a complete solution to the control system design problem. The solution to this problem may not exist if the system considered is not controllable. Although most physical systems are controllable and observable, the corresponding mathematical model may not possess the properties of controllability and observability. In this case it is necessary to know the conditions for a system to be controllable and observable.

1.5.4 Stability

Stability is a very important concept in system control theory, that is, under what conditions will a system become unstable? If it is unstable, how should we stabilize the system? Whether or not a system is stable is a property of the system itself and does not depend on the input or driving function of the system.

Stability is also one of the hardest function properties to prove. There are several different criteria for system stability, but the most common requirement is that the system must produce a finite output when it is subjected to a finite input.

1.5.5 Convergence

Convergence refers to the notion that some functions and sequences approach a limit under certain conditions.

There is a difference between classical control theory and quantum control theory: probability is the control objective of quantum systems, which means the control goal is not achievable completely for a stable control system with non-zero error. For this reason, a convergent control with zero error is required in quantum control systems. In summary, a mature quantum control theory is able to not only manipulate various states of particular needs, but also to design a convergent control law.

1.5.6 Robustness

A control system must always have some robustness. A robust control system is one in which the performance does not change much if the actual system is slightly different from the mathematical model used for the synthesis and controller design. This specification is important: no real physical system truly behaves like the series of differential equations used to represent it mathematically. Typically, a simpler mathematical model is chosen in order to simplify the calculation because the true system dynamics can be so complicated that a complete model is impossible.

1.6 Performance of Control Systems

1.6.1 Probability

A quantum system can be in two possible states, for example the polarization of a photon. When the polarization is measured, it could be horizontal, labeled as state $|H\rangle$, or vertical, labeled state $|V\rangle$. Until its polarization is measured, the photon can be in a superposition of both these states, so its wave function $|\psi\rangle$ would be written:

$$|\psi\rangle = \alpha |H\rangle + \beta |V\rangle$$

The probability amplitudes of states $|H\rangle$ and $|V\rangle$ are α and β , respectively. When the photon's polarization is measured, the system is horizontally polarized with probability $|\alpha|^2$ and vertically polarized with probability $|\beta|^2$. Therefore, a photon with the wave function $|\psi\rangle = \sqrt{\frac{1}{3}}|H\rangle + i\sqrt{\frac{2}{3}}|V\rangle$, whose polarization is measured, would have a probability of $\frac{1}{3}$ to be horizontally polarized and a probability of 2/3 to be vertically polarized. The measurement must give either $|H\rangle$ or $|V\rangle$, so the total probability of measuring $|H\rangle$ and $|V\rangle$ must be 1. This leads to a constraint that $|\alpha|^2 + |\beta|^2 = 1$; more generally, the sum of the squared moduli of the probability amplitudes of all the possible states is equal to 1. The wave function that fulfills this constraint is called the normalized wave function.

The probability amplitude interprets the physical meaning of the wave function. In quantum mechanics, a probability amplitude is a complex number whose modulus squared represents a probability or probability density. For example, if the probability amplitude of a quantum state is α , the probability of measuring that state is $|\alpha|^2$. The values taken by a normalized wave function ψ at each point *x* are probability amplitudes, since $|\psi(x)|^2$ gives the probability density at position *x*.

1.6.2 Fidelity

In quantum information theory, the fidelity is a measure of the "closeness" of two quantum states. It is not a metric on the space of density matrices, but it can be used to define the Bures metric on this space.

Definition 1.1 Given two density matrices ρ and σ , the fidelity is defined by

$$F(\rho,\sigma) = Tr\left[\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}}\right]$$

By $M^{1/2}$ of a positive $\rho = |\phi\rangle\langle\phi|$ semi-definite matrix M we mean its unique positive square root given by the spectral theorem. The Euclidean inner product from the classical definition

is replaced by the Hilbert–Schmidt inner product. When the states are classical, that is, when ρ and σ commute, the definition coincides with that for probability distributions.

An equivalent definition is given by

$$F(\rho,\sigma) = \|\sqrt{\rho}\sqrt{\sigma}\|_{tr}$$

where the norm is the trace norm (sum of the singular values). This definition has the advantage that it clearly shows that the fidelity is symmetric in its two arguments.

Some examples follow.

1. Suppose that one of the states is pure: Then $\sqrt{\rho} = \rho = |\phi\rangle\langle\phi|$ and the fidelity is

$$F(\rho,\sigma) = Tr\left[\sqrt{|\phi\rangle\langle\phi|\sigma|\phi\rangle\langle\phi|}\right] = \sqrt{\langle\phi|\sigma|\phi\rangle}Tr\left[\sqrt{|\phi\rangle\langle\phi|}\right] = \sqrt{\langle\phi|\sigma|\phi\rangle}$$

If the other state is also pure, $\sigma = |\psi\rangle\langle\psi|$, then the fidelity is

$$F(\rho,\sigma) = \sqrt{\langle \phi | \psi \rangle \langle \psi | \phi \rangle} = |\langle \phi | \psi \rangle|.$$

This is sometimes called the overlap between two states. If, say, $|\phi\rangle$ is an eigenstate of an observable, and the system is prepared in $|\psi\rangle$, then $F(\rho, \sigma)^2$ is the probability of the system being in state $|\phi\rangle$ after the measurement.

2. Let ρ and σ be two density matrices that commute with each other. They can therefore be simultaneously diagonalized by unitary matrices, and we can write

$$\rho = \sum_{i} p_{i} |i\rangle \langle i| \text{ and } \sigma = \sum_{i} q_{i} |i\rangle \langle i|$$

for some orthonormal basis $\{|i\rangle\}$. Direct calculation shows the fidelity is

$$F(\rho,\sigma) = \sum_{i} \sqrt{p_i q_i}$$

This shows that, heuristically, the fidelity of quantum states is a genuine extension of the notion from probability theory.

1.6.3 Purity

In quantum mechanics, and especially quantum information theory, the purity of a state is a scalar defined as

$$\gamma = Tr(\rho^2)$$

where ρ is the density matrix of the state.

For the closed quantum system, the purity of a pure state is always equal to 1, that is, $Tr(\rho^2) = 1$, while the purity of a mixed state is less than 1, that is, $Tr(\rho^2) < 1$.

The purity is trivially related to the linear entropy S_L of a state by

$$\gamma = 1 - S_L$$

1.7 Quantum Systems Control

1.7.1 Description of Control Problems

The greatest advantage of a control law designed according to system control theory is that one can design a better or OC law and determine its parameters by the control theory instead of by tentative experiments. The control law derived from theory will lead an experiment to its desired results. In this sense, the design of the control law is the task of finding the best parameters according to some control theory, which results in many challenges for quantum control engineering:

- 1. It is not always a convex optimization problem.
- 2. The space to be searched for optimization is always infinite: it can be defined in either a finite $[0, t_f]$ or an infinite $[0, \infty)$ interval. In practice, one way to reduce optimization space is to obtain a finite-dimensional solution with control parameters that is the most common one and can be realized by means of smoothing constant function approximation.
- 3. To solve partial differential equations, a time-consuming computation is needed.
- 4. It is difficult to solve the equation of a controlled system in a non-standard form.
- 5. The model of a controlled system is less accurate.

The parameterized control field in a general form is $u(t) = \sum_{m=1}^{M} a_m \cos(\omega_m t + \phi_m)$, where a_m ,

 ω_m , and ϕ_m are parameters to be optimized according to the control theory. The most typical problem in a quantum system is to design a set of control functions $u_m(t)$, m = 1, ..., M, to steer the system from its initial state to a desired target one. For unitary evolution in a Hamiltonian system, the frequency spectrum of $\rho(t)$ is time-independent or $Tr[\rho^n(t)] = Tr[\rho_0^n(t)], \forall n \in 1, ..., N$. That is to say, to make sure the target state ρ_f is achievable, the same frequency spectrum (or entropy) is used for both ρ_0 and ρ_f . The system is controllable for its density matrix. If the entropies of ρ_0 and ρ_f are different from each other, one can minimize the distance index $\|\rho(t) - \rho_f(t)\|$ to accomplish the control task.

It can be shown that ρ_f is stationary under the condition that ρ_f and H_0 are commutable, viz. $[H_0, \rho_f(0)] = 0$. Thus, quantum state control for most target states is a problem of the transfer. For a non-stationary target, it is a trajectory tracking problem: find a function u(t) to make a trajectory of $\rho(t)$ with initial state ρ_0 track the target trajectory of $\rho_f(t)$. In the latter case, the problem may need to distinguish trajectory tracking. Both orbit tracking and functional tracking exist in quantum systems. It is considered that $\rho(t)$ itself is a trajectory and the target state ρ_f evolves according to its own orbit. The orbit is expressed as the globe phase of the quantum state, which does not influence the states' amplitude and does not need to be considered. In both orbit and functional tracking, the trajectory of $\rho(t)$ is a time-dependent function and can be decided by the control value.

1.7.2 Quantum Control Theory and Methods

Quantum control theory is a rapidly developing research area. Controlling quantum phenomena has been an implicit goal in much quantum physics and chemistry research since the establishment of quantum mechanics (Warren, Rabitz, and Dahleh, 1993; Chu, 2002). One of the main goals in quantum control theory is to establish a firm theoretical footing and develop a series of systematic methods for the active manipulation and control of quantum systems (Mabuchi and Khaneja, 2005). This goal is non-trivial since microscopic quantum systems have many unique characteristics (e.g., entanglement and coherence) which do not occur in classical mechanical systems and the dynamics of quantum systems must be described by quantum theory. In recent years, the development of the general principles of quantum control theory has been recognized as an essential requirement for the future application of quantum technologies (Dowling and Milburn, 2003).

Similar to macroscopic control systems, we can divide quantum control systems into two classes: state transfer and trajectory tracking. The former can be subdivided into control of pure states and general states. Many kinds of control methods have been proposed for every control problem. Each control method has its own characteristics and a range of suitable applications. Among the different control methods there are certain differences in the amount of computation, the performance of the solution and the degree of difficulty of the realization. A complete control process of quantum systems involves choosing the proper system model to be controlled and designing a control strategy to reach the desired control goal, which requires knowledge of various mathematical models and related control theories.

Generally, the premise to design a controller for a system is the system's controllability, otherwise the desired output state cannot be achieved by any control input. The controllability of the controlled system must therefore be studied before designing a controller. The controllability conditions themselves only provide the criterion to determine whether or not a system is controllable and do not take a part in the controller design. The basic condition required so that the controller designed by a control theory can be used is stability of the whole control system. If the controlled system is not only stable but also convergent, the error between the reference and the controlled system will be zero. The stability can only guarantee an allowable error range, not the convergence. However, a convergent system must be stable. So far controllability in quantum control theory has received much attention and great progress has been made, especially for finite-dimensional closed quantum systems.

It is worth noting that automatic control systems have been widely used in physical experiments for a long time. Between the late 1980s and the early 1990s, ultrafast lasers, so-called femtosecond lasers, appeared along with the rapid development of laser industry. This new generation of lasers has the ability to generate pulses with durations of a few femtoseconds $(1 \text{ fs} = 10e^{-15} \text{ seconds})$ and even less. The duration of such a pulse is comparable with the period of a molecule's natural oscillation, therefore a femtosecond laser can, in principle, be used as a means of controlling a single molecule or atom. A consequence of such an application is the possibility of realizing the chemist's dream of changing the natural course of chemical reactions. In addition, control is an important part of many recent nanoscale applications: nanomotors, nanowires, nano chips, nano robots, and so on. Using the apparatus of modern control theory, new horizons in studying the interactions of atoms and molecules may bring new ways and possible limits for the intervention in intimate processes of the micro-world.

Many control methods and technologies for systems have been proposed. The easiest one is π pulses dynamics, different pulse areas of which in resonant single-photo transition or resonant double-photos Raman transition are used to build coherent states. This can realize the complete population overturn of a two-level system but comes with the difficulties of accurate control of pulse intensity and duration time. Based on adiabatic theory, some manipulation technologies have been proposed and realized, such as Chirped Adiabatic Passage (CHIRAP)

and Stimulated Raman Adiabatic Passage (STIRAP). In both of these the adjustment of pulse parameters such as frequency, amplitude envelope, and so on is extremely slow to make the transition go along adiabatic defined dressed states. The strategy is expected to achieve complete population transfer of the target state. In view of the facts mentioned above, it is very difficult to apply these theories to more general needs such as the control of a superposition state or a mixed state. Furthermore, control law is based on the feedback of measure, where measurement is described by measure operators. In general, the reliability of measure operators is a serious problem that feedback control has to face.

Among the control methods based on control theories, quantum OC based on optimal control theory (OCT) is the most successful, and turns the problem of state manipulation into the one of global optimization. In the OC approach, the quantum control problem can be formulated as a problem of seeking a set of admissible controls satisfying the system dynamic equations and simultaneously minimizing a cost functional. The cost functional may be different according to the practical requirements of the quantum control problems, such as minimizing the control time and the control energy, the error between the initial state and target state, or a combination of these requirements. Many useful tools in traditional OC, such as the variational method, the Pontryagin minimum principle, and convergent iterative algorithms, can be adapted to quantum systems and applied to search for OCs. OC techniques have been widely applied to control quantum phenomena in physical chemistry and NMR experiments. In such a control method, time-independent performance functions are more flexible and suitable for diverse optimal problems, but the main weakness of these is that the optimal problem is a two-point boundary value problem, and the evolution of system dynamical equations and their states depend on the initial control field. One has to guess an initial value to start the design process of the control field and to optimize by continuous iterations. This requires a large amount of computing, which limits its application to quantum physics, where a rapid response is needed.

Lyapunov-based control methods are powerful tools for feedback controller design in classical control theory (Dong and Petersen, 2010). In quantum control, the acquisition of feedback information through measurements usually destroys the state being measured, which makes it difficult to directly apply Lyapunov approaches to quantum feedback controller design. However, one may first complete the feedback control design by simulation on a computer, which will give a sequence of controls, then apply the control sequence to the quantum system to be controlled in an open-loop form (Mirrahimi, Rouchon, and Turinici, 2005; Kuang and Cong, 2008). This is a feedback design and open-loop control strategy at the current level of technology. This strategy is especially useful for some difficult quantum control tasks (Altafini, 2007). The most important aspects of Lyapunov-based control design are the construction of the Lyapunov function, the determination of the control law, and the analysis of the convergence.

The advantage of the Lyapunov-based method is that control law can be obtained directly from the Lyapunov indirect stability theorem without iterations from the solution of partial differential equations, which makes it possible to realize rapid quantum control. The main shortcoming of the Lyapunov-based method is that it is usually only a stable control method, not a convergent control method. A given target state requires the control system to be convergent to guarantee that the system achieves the desired target state. To achieve this goal the convergence of the Lyapunov-based method has been studied intensely in recent years.

Bang-bang control and geometry control are alternative control methods often used in quantum systems. Geometry control is suitable for lower level systems, especially when combined with the Bloch sphere, which can help the physical meaning of the quantum state in a two-level system to be understood. The trajectory of geometry control of a pure state in two-level systems is just the trajectory on a Bloch sphere, while the trajectory of the mixed state is the points inside the Bloch sphere. The bang-bang control in control theory is a type of simple switch control, which corresponds to the pulse control in quantum systems. Because of its simple realization, bang-bang control was used earlier in quantum systems. In open quantum systems several special control theories and methods have been developed, such as the decoherence-free subspace (DFS) method and the dynamic decoupling quantum control method.

All of the quantum control theories and methods mentioned above are covered in this book. There are important differences between quantum control theory and its experimental implementation. Control solutions obtained from theoretical studies strongly depend on the employed model Hamiltonian. However, for real systems controlled in the laboratory, the Hamiltonians usually are not well known (except for the simplest cases) and the Hamiltonians for the system-environment coupling are known to an even lesser degree. An additional difficulty is the computational complexity of accurately solving the OC equations for realistic polyatomic molecules. Another important difference between control theory and experiment arises from the difficulty of reliably implementing theoretical control designs in the laboratory because of instrumental noise and other limitations. As a result, optimal theoretical control designs generally will not be optimal in the laboratory. Notwithstanding these comments, control simulations continue to be very valuable and they even set forth the logic leading to practical laboratory control.

1.8 Overview of the Book

This book presents the latest developments and achievements in control theories and methods in both closed and open quantum systems. The contents are suitable for both active researchers and non-experts who wish to enter the field. Each chapter discusses how to use and design the particular control method or theory, which types of systems can use it, and what information can be learned from the control system. Some possible further developments and extensions of the methods that may be expected in the near future are also mentioned. The book places an emphasis on ideas and concepts, with a fair to moderate amount of mathematical rigor. The simulation experiments and results display all essential information about the quantum state under the control methods used and will greatly enhance the reader's understanding of quantum mechanics and the effectiveness of control theories.

The book can be divided into two parts: control theory and methods for closed and open quantum systems. Chapter 1 is provides an introduction to the subject. Chapters 2–9 cover control methods for closed quantum systems, and Chapters 10–14 cover control methods for open quantum systems. Chapter 15 discusses the trajectory tracking of quantum systems. In the control theory and methods for the closed quantum systems section, Chapters 4–8 concentrate on quantum control theory based on the Lyapunov method.

The book is organized as follows.

We begin the basic analysis of system states in a simple two-level quantum system on the Bloch sphere in Chapter 2. We also introduce the state transfer of quantum systems on the Bloch sphere by means of geometric control. The Bloch sphere is a suitable tool used to present a qubit because it gives us an intuitive vision to understand the physical meanings of quantum bits or variables. We first present the descriptions of pure states, superposition states, and mixes states. Then we propose the control methods of a single spin-1/2 particle in a Bloch sphere in which we focus on the situations of a minimum control field and a fixed time *T*, respectively.

Chapter 3 is about the general control methods of closed quantum systems. Two improved OC strategies applied to quantum systems are presented first. After that the design of the control sequence of pulses for a high-dimensional spin-1/2 quantum system is used to prepare the entangled state. Chapter 3 also provides a comparison study between geometric control and bang-bang control, which are the two earliest control methods used in quantum systems.

Chapters 4–8 introduce quantum control theory based on the Lyapunov method. The first three chapters are the Lyapunov methods that are used in state transfer between diverse quantum states. They are the manipulation of eigenstates, population control, and general state control, respectively. Chapter 7 covers the convergence analysis of the Lyapunov method. The Lyapunov method is discussed in so many chapters because this method is an increasingly interesting method used in quantum control systems. It will be applied in quantum systems as it is in control engineering applications. From the convergence conditions obtained in Chapter 7, it can be seen that the convergence conditions are so strong that most practical systems are not able to satisfy them. In order to relax the convergence conditions to comply with actual cases, we specifically introduce control theory and method in degenerate cases in Chapter 8.

Chapter 4 introduces the eigenstates transfer control law design process for the selected Lyapunov function based on the state distance according to the Lyapunov stability theorem. We also present an optimal quantum control based on the Lyapunov stability theorem, and the realization of the quantum Hadamard gate based on the Lyapunov method.

There are three parts in Chapter 5: the population control of equilibrium states, the generalized control of quantum systems in the frame of vector treatment, and the population control of eigenstate and its simulation.

Chapter 6 covers the general state control method in quantum systems, including superposition state manipulation, pure state control strategy, and the OC of the mixed state, and from any pure state to mixed state manipulation.

Chapter 7 focuses on the convergence analysis of the Lyapunov-based method. This chapter starts with the mathematical expressions of invariant set and then gives the analysis of invariant set based on the connectivity graph of energy levels. For the diagonal Lyapunov function, the construction and adjustment principles of diagonal elements are presented. The initial state is also considered. A necessary and sufficient convergence condition is introduced and strict proof of convergence will be presented. For the case where the convergence condition is not satisfied, a path programming the control strategy of the quantum state transfer is presented to solve the problem.

Quantum control systems that do not satisfied the necessary and sufficient convergence conditions are called non-degenerate cases. Chapter 8 deals with these kinds of control systems. For this purpose, an implicit Lyapunov function is introduced, and an implicit Lyapunov control approach to multi-control Hamiltonians systems based on state error and an implicit Lyapunov control approach based on the average value are presented.

Chapter 9 covers the manipulation methods of the general state and studies three alternative situations: quantum system Schmidt decomposition and its geometric analysis, the preparation of entanglement states in a two-spin system, and the purification of a mixed state for two-dimensional systems.

Chapters 10–14 present the control methods of open quantum systems, with Chapter 10 concentrating on the presentation of general control methods. Chapter 11 covers state estimation, measurement, and control of quantum systems, and Chapter 12 covers the control method of state preservation. Chapter 13 explains state manipulation in the DFS and Chapter 14 covers dynamic decoupling quantum control methods. The specific contents of these five chapters are as follows.

The states transfer of open quantum systems with a single control field is presented in Chapter 10. In the simulations, the free evolution of the system without the external control and system behavior under the control action are compared. Two cases are studies: in one the target states are equilibrium states of the system to be contolled and in the other some mixed states are examined. Chapter 10 also introduces purity and coherence compensation by the interactions between particles.

The state estimation methods in quantum systems are presented in Chapter 11. The state estimation methods introduced include the quantum state estimation method based on measuring the identical copy of the system, state topography, the maximum entropy estimation method, the maximum likelihood (ML) estimation method, the Bayesian method, the minimum variance (least square-variance, LS) estimation method, and the quantum state reconstruction method. We also introduce entanglement detection and measurement of quantum systems, which include entangled state representation, separation criterion, entanglement witnesses in experiments, entanglement quantization, entanglement degree of a multi-body system, the estimation of entanglement degree, and non-linear separation criteria. Finally in Chapter 11 we present decoherence control based on weak measurement.

Chapter 12 highlights state preservation of open quantum systems. The coherence preservation in a Λ -type three-level atom, the purity preservation of quantum systems by resonant field, and the coherence preservation in Markovian open quantum systems are studied.

In the study of state manipulation in the DFSs in Chapter 13, the construction of DFS which contains the desired target state is presented first, then the Lyapunov-based method in the interaction picture is designed. Three simulation experiments are implemented in a three-level Λ -type quantum system, a four-level energy open quantum system, and a Λ -type *N*-level atomic system.

Dynamic decoupling is a special control method in open quantum systems. In Chapter 14 we present the phase decoherence suppression in an arbitrary *n*-level atom in ξ -configuration with bang-bang controls, the optimized DD in an ξ -type *n*-level atom, and an optimized DD strategy to suppress decoherence. This chapter should help the reader to have a better understanding of the dynamic decoupling quantum control method.

Chapter 15 covers the trajectory tracking of quantum systems, which is another type of control relative to state transfer (regulation) control. We focus on orbit tracking control of closed quantum systems. In the numerical simulation experiments and results analyses, we explain tracking control between eigenstates, between superposition states, between eigenstates and superposition states, and between superposition states and eigenstates. We propose an adaptive trajectory tracking of quantum systems. We also study the convergence of orbit tracking for quantum systems in which several cases and problems, including diagonal target states and non-diagonal target density matrices, are considered and solved.

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