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Liouville-space-based optimal control modeling of quantum system

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ABSTRACT

We investigate the modeling of optimal control of quantum system in Liouville space by combining classical engineering control theory with quantum theory. Aiming at two typical models of optimal control, we derive the requirements of optimal control via taking the expected value of the observable physical quantity to maximum as performance index, which forms the bedrock for further investigating the design of control law.

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1. Introduction

Quantum information technologies are composed of quantum computation, quantum communication and quantum control [1–5]. Combining the principles of quantum mechanics and approaches of classical engineering control, quantum control implement controlling on the states of quantum system by means of electrical field, magnetic field or electromagnetic field. From 1980s, researchers have made foundational work in modeling of quantum control, controllability analysis and observability [6–8]. For the closed quantum system, people adopt the strategies of open-loop control, optimal control, learning control and feedback control to realize quantum control, and the research results achieved have successfully been applied in quantum inform, quantum chemistry, laser cooling and new nanotechnology, etc. [9].

Quantum manipulation is essential for quantum information processing, and the investigation of control strategy is most important in quantum control. Presently, the control strategies mainly involve learning control, feedback control, optimal control and Lyapunov control. Close-loop control should have become the preferred approach in controlling complicated quantum system; however, open-loop control remains the major method for implementing open quantum system control owing to the unobservability of quantum states and the limitations of feedback control. The optimal control plays significant role in quantum open-loop control, based on which people have proposed the optimal control of population, optimal control of time and optimal control of energy for the open quantum system. Ref. [10] discussed the strategy of utilizing the optimal control of middle bath model to suppress decoherence. Up to now, however, the research on discussing decoherence suppression with the method of optimal control is seldom [11,12]. In previous work, Rabitz succeeded in designing optimal control field and carrying out much research based on optimal control theory [13,14]. In most present research of optimal control, however, the subjects investigated are simple and low-dimensional physical systems, forcing people neglect the effect of other dimension on the controlling process and result, which is practically unfavorable for the decoherence control in quantum system.

In this paper, we investigate the modeling of quantum system under optimal control in quantum Liouville space. Aiming at two typical models of quantum optimal control, we derive the requirements of optimal control via taking the expected value of the observable physical quantity to maximum as performance index.

2. Theory model

The state of quantum system can be described by many ways. When the system is in pure state, it can be described by the wave function that evolves according to Schrodinger equation. The density operator $\hat{\rho}(t)$ can also be used and is more convenient under many conditions. It cannot only denote pure state but also denote mixed state, especially can conveniently extend to infinite dimensional physical space. Therefore, the density operator $\hat{\rho}(t)$ is adopted to represent the state of system. In the Hilbert space $\hat{H}(t)$,

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the dynamical evolution of the system state satisfies the quantum Liouville equation.

$$i\hbar\frac{\partial}{\partial t}\hat{\rho}(t)=[\hat{H}(t),\hat{\rho}(t)]. \tag{1}$$

In the problem of optimal control in quantum system, the extremum track must satisfy the state equation of the system. Therefore, from a mathematical point of view, quantum optimal control is namely the constrained functional extremum problem.

Generally, the description of quantum state is constructed in Hilbert space. Whereas when the density operator $\hat{\rho}(t)$ is used to describe the state evolution, it is more convenient to extend Hilbert space to Liouville space. Each linear operator $\hat{A}$ in Hilbert space corresponds to a vector $|\hat{A}\rangle\rangle$ in Liouville space. Then, the quantum Liouville equation in Liouville space can be written as

$$i\hbar\frac{\partial}{\partial t}|\hat{\rho}(t)\rangle\rangle=\hat{\ell}(t)|\hat{\rho}(t)\rangle\rangle, \tag{2}$$

where $\hat{\ell}(t)\hat{\rho}(t)\equiv[\hat{H}(t),\hat{\rho}(t)]$ is called Liouville super operator.

The control on quantum system is realized usually through interacting the externally applied optical field or electromagnetic field with the dynamical variables of the system, which is equivalent to introduce some Hamiltonian into the original Hamiltonian to change the energy of the system. It is called coherent control since such control way can keep the coherence invariant. Under coherent control, the Hamiltonian is given as

$$\hat{H}(t)=\hat{H}_0+\hat{H}_c(t). \tag{3}$$

where $\hat{H}_0$ represents the original Hamiltonian of the controlled quantum system and is usually time-independent. $\hat{H}_c(t)$ denotes the interacting Hamiltonian between the control field and controlled quantum system.

From the state parameter point of view, the control problem of quantum system can be described as the problem of state transfer. From the quantum measurement point of view, it is the problem of expected value for a specified observable physical quantity. The quantum state described by quantum mechanics is abstract mathematical description and lacks any observable physical connotation. Therefore, people are more interested in the time variation of the observable physical quantity than that of the quantum state. The control theory relies on measurement. Only the state performance of the system is real-time known, the real-time control can be realized. In this work, we mainly focus on the expected value of the observable physical quantity. The performance index is taken as

$$\mathrm{Max}J=\langle\langle\hat{A}|\hat{\rho}(t_f)\rangle\rangle-\int_{t_0}^{t_f}F[u(t),t]\,dt. \tag{4}$$

which is an aggregative indicator. The first term represents the average value of specified observable physical quantity at the terminal time, and the second one closely relates with the externally applied controlling parameter. It possesses explicit physical connotation that the average value of specified observable physical operator $\hat{A}$ is maximum at the terminal time. Obviously, such aggregative indicator is the Bolza problem in optimal control.

3. Euler–Lagrange equation under the strategy of optimal control

Applying the theory of optimal control to manipulate the physical systems require to determine the form of performance index and control the tolerance of action based on the given state equation and the boundary conditions. In this section, taking the expected value of the observable physical quantity to maximum as performance index, we propose the requirements for the optimal control under the given initial time and initial state, namely focus on the Euler–Lagrange equation under the strategy of optimal control.

3.1. The terminal time t_f is given and the terminal state $|\hat{\rho}(t_f)\rangle\rangle$ is optional

Practically, the processing of quantum information should be completed in very limited time since the quantum system is extremely easy to be influenced by external environment including the measuring apparatus that leads to decoherence. It is namely the foundation for the physical model that the terminal time is given and the terminal state is optional.

Firstly, we introduce the n-dimensional Lagrange operator $\lambda(t)$:

$$\langle\langle\lambda(t)|=(\,\lambda_1^*(t)\quad\lambda_2^*(t)\quad\cdots\quad\lambda_n^*(t)\,). \tag{5}$$

which is a time-dependent function corresponding to dynamic optimal problems. Combining with Eq. (4), the Lagrange function is given as

$$L=\langle\langle\hat{A}|\hat{\rho}(t_f)\rangle\rangle-\int_{t_0}^{t_f}F[u(t),t]\,dt-\int_{t_0}^{t_f}\left\langle\left\langle\lambda(t)\right|\left[\frac{\partial}{\partial t}-\frac{1}{i\hbar}\hat{\ell}(t)\right]\left|\hat{\rho}(t)\right\rangle\right\rangle dt. \tag{6}$$

By using subsection integration to solve the third term in the right hand of above formula, the Lagrange function can be rewritten as:

$$L=\langle\langle\hat{A}|\hat{\rho}(t_f)\rangle\rangle-\langle\langle\lambda(t_f)|\hat{\rho}(t_f)\rangle\rangle+\langle\langle\lambda(t_0)|\hat{\rho}(t_0)\rangle\rangle-\int_{t_0}^{t_f}F[u(t),t]\,dt+\int_{t_0}^{t_f}\left\langle\left\langle\lambda(t)\right|\frac{1}{i\hbar}\hat{\ell}(t)\left|\hat{\rho}(t)\right\rangle\right\rangle dt+\int_{t_0}^{t_f}\left\langle\left\langle\frac{d\lambda(t)}{dt}\,\right|\hat{\rho}(t)\right\rangle\right\rangle dt. \tag{7}$$

In this paper, superscript "∼"denotes the optima of corresponding state parameters or mechanical quantities, such as $\tilde{\hat{\rho}}(t)$, $\tilde{u}(t)$, $\tilde{t}_f$ is respectively the optimum of $\hat{\rho}(t)$, $u(t)$, t_f. Notice that when t_f is given, the variation of Eq. (7) is caused by $\delta|\hat{\rho}(t)\rangle\rangle$, $\delta|\hat{\rho}_f(t)\rangle\rangle$, $\delta|\lambda(t)\rangle\rangle$ and δu. Then we obtain:

$$\delta L=\frac{\partial L}{\partial|\hat{\rho}(t)\rangle\rangle}\delta|\hat{\rho}(t)\rangle\rangle+\frac{\partial L}{\partial|\lambda(t)\rangle\rangle}\delta|\lambda(t)\rangle\rangle+\frac{\partial L}{\partial|\hat{\rho}(t=t_f)\rangle\rangle}\delta|\hat{\rho}(t_f)\rangle\rangle+\frac{\partial L}{\partial u}\delta u. \tag{8}$$

Utilizing the operator formulae in Liouville space:

$$\langle\langle\hat{A}|\hat{B}\rangle\rangle^*=\langle\langle\hat{B}|\hat{A}\rangle\rangle,\quad\langle\langle\hat{A}|\hat{C}|\hat{B}\rangle\rangle=\langle\langle\hat{B}|\hat{C}^+\hat{A}\rangle\rangle$$

and combining with Eq. (2), after straightforward but complicated deduction, we obtain

$$\frac{\partial L}{\partial|\hat{\rho}(t)\rangle\rangle}=\int_{t_0}^{t_f}\left[\frac{d}{dt}-\frac{1}{i\hbar}\hat{\ell}(t)|\lambda(t)\rangle\rangle\right]^*dt, \tag{9}$$

$$\frac{\partial L}{\partial\left|\lambda(t)\right\rangle\rangle}=\left[\frac{\partial}{\partial t}-\frac{1}{i\hbar}\hat{\ell}(t)\right]\left|\hat{\rho}(t)\right\rangle\rangle, \tag{10}$$

$$\frac{\partial L}{\partial|\hat{\rho}(t=t_f)\rangle\rangle}=\left[|\hat{A}\rangle\rangle-|\lambda(t_f)\rangle\rangle\right]^*. \tag{11}$$

The prerequisite of the Lagrange function L taking maximum is that the variation of δL is zero for arbitrary $\delta|\hat{\rho}(t)\rangle\rangle$, $\delta|\hat{\rho}_f(t)\rangle\rangle$, $\delta|\lambda(t)\rangle\rangle$ and δu. Then the following relations that the optimum satisfies are obtained:

$$i\hbar\frac{\partial}{\partial t}|\tilde{\hat{\rho}}(t)\rangle\rangle=\hat{\ell}(t)|\tilde{\hat{\rho}}(t)\rangle\rangle, \tag{12}$$

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