ABSTRACT

ZHANG, QIN. Control of Infinite Dimensional Bilinear Systems: Applications to Quantum Control Systems. (Under the direction of Dr. Kazufumi Ito).

In the dissertation, optimal control problem for bilinear systems motivated from quantum control theory are studied. Specifically, problems of quantum feedback control, control of tumor growth dynamics and time optimal control are analyzed for bilinear systems. Feedback synthesis, receding horizon synthesis and semi-smooth Newton method are developed to solve these problems. The contents of the dissertation are outlined as follows:

The first problem studied is control of quantum systems described by the linear Schrödinger equation. Control inputs enter through coupling operators and results in a bilinear control system. Feedback control laws with switching term are developed for the orbit tracking and the performance of the feedback control laws is demonstrated by a stable and accurate numerical integration of the closed-loop system. The asymptotic properties of the feedback laws are analyzed by the LaSalle-type invariance principle. The receding horizon control synthesis is applied to improve the performance of the feedback law. The second order accurate numerical integrations via time-splitting and the monotone convergent iterative scheme are combined to solve the optimality system.

The switching mechanism in the feedback law can be applied to a wide general class of control systems and feedback synthesis based on the Lyapunov stability. By using this principle, the problem of the tumor treatment, aiming at the reduction of the tumor cells population, is formulated in terms of optimal control theory as a state regulator problem and a feedback law with switching term is designed. Numerical evidence is shown to demonstrate the effectiveness of the feedback law to suppress the tumor growth.

A quantum system interacts with its environment. As a consequence, quantum state subject to continuous measurement can be modeled as a nonlinear stochastic differential equation by quantum filtering theory. The problem of stochastic stabilization of quantum spin systems under the noisy environment and continuous measurement via feedback control is studied. New nonlinear control law with switching term is proposed and developed to globally stabilize the quantum spin system to an arbitrary equilibrium state. Nonnegative definite preserving properties of the density matrix to measure the quantum system is very essential and a numerical method is developed to fulfill this.

Finally, time optimal and minimum effort control problems for linear and bilinear systems are studied. To overcome the difficulties of nondifferentiability in the bang-bang control, a regularized problem is formulated and the semi-smooth Newton method is applied for solving the regularized optimality system. By integrating the state and costate and variation of them in the optimality system, the nonlinear optimality system is further reduced to a nonlinear equation with some shooting parameters. The reduced Jacobian is computed for the Newton update. The initialization of the Newton method is achieved by solving a related minimum norm problem and using the standard line search strategy. The effectiveness of the proposed method is demonstrated by examples for quantum spin system and parabolic systems.

Control of Infinite Dimensional Bilinear Systems: Applications to Quantum Control Systems

by
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DEDICATION

To my parents, Shunquan Zhang and Lanying Wu

BIOGRAPHY

Qin Zhang was Born in Shanghai, China on August 18th, 1981. He spent his childhood at Liangshan, a small town in Xinyu City, Jiangxi Province, China. At age of fifteen, he went back to Shanghai and attended North District Middle School, then Fuxing High School. Starting year 1999, he attended Fudan University to study mathematics. Upon graduation, he went to the United States to have his graduate study. He received his master degree in mathematics at the University of Toledo in 2005. Starting from Fall 2005, Qin spent his life at North Carolina State University pursuing his Ph.D degree in applied mathematics.

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Chapter 1

Introduction

In the dissertation, we study the bilinear control system of the form

$$\frac{dx(t)}{dt} = Ax(t) + Bu(t)x(t) \tag{1.1}$$

where $x(t) \in X$ is the state variable, $u(t) \in U$ is the admissible control. A is a linear operator on X and B is the input operator from U to X. (1.1) is called bilinear since its right side is a linear function of the state $x(t)$ and the control $u(t)$. Typical examples for the bilinear system (1.1) arise in quantum control problem and tumor growth model.

1.1 Overview of Quantum Control Problem

Since the first advent of the laser in 1960's, physicists and chemists had the vision to coherently control quantum systems using laser fields. Throughout years, the inquiries of modern science and the demands of advancing technology are driving theoretical and experimental research towards control of quantum systems. Wide areas of application for quantum control have been studied and implemented . For instance, control and identification of chemical reactions in quantum chemistry [58], [57], protein structure determination via nuclear magnetic resonance (NMR) [20] [51], quantum information and quantum computing [50], quantum optics, and so on. A good review is [42].

In many experimental setups, an electromagnetic field interacts with a quantum system, such as an atom, a nucleus or an electron, whose dynamics follows the laws of quantum mechanics. By semiclassical approximation, the control field, that is, the electromagnetical field influencing the quantum system is taken to be a classical source. Then the dynamics of state of a quantum system $\Psi(x,t)$, represented by a vector in a Hilbert space H can be modeled by the Schrödinger equation,

$$i\frac{d}{dt}\Psi(x,t) = (\mathcal{H}_0 + \epsilon(t)V)\Psi(x,t) \tag{1.2}$$

where the internal Hamiltonian $\mathcal{H}_0$ describes the internal dynamics of the system. The control Hamiltonian V describes coupling of the system with the interacting electromagnetical field $\epsilon(t)$. The Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \epsilon(t)V$ represents the total energy of the system. The system (1.2) are called bilinear, since the Hamiltonian is a linear function of both the state $\Psi(x,t)$ and the control $\epsilon(t)$.

Now we present two examples of the quantum system. The first one is Spin-$\frac{1}{2}$ system, which is in a finite dimensional state space. It is used to describe the dynamics of a single particle with spin. In quantum mechanics, spin is a fundamental property of atomic nuclei, hadrons, and elementary particles. It corresponds to an internal angular momentum of the particle. Particles, such as the electron, positron, neutron and quake all have spin-$\frac{1}{2}$. To describe the dynamics of spin-$\frac{1}{2}$ system, the state space is set to be $\mathbb{C}^2$ and the Hamiltonian is given by

$$\mathcal{H} = -\gamma \sum_{i=x,y,z} S_i B_i \tag{1.3}$$

for some proportionality factor γ called the gyromagnetic ratio, where B_x, B_y, B_z are the components of the magnetic field at the position of the particle and S_x, S_y, S_z are the spin operators, which are 2×2 Hermitian matrices. They are simply expressed in terms of the Pauli matrices,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{1.4}$$

as $S_i = \frac{1}{2}\sigma_i$. In most applications, a large uniform, constant magnetic field B_0 is applied in one direction (say z). The reason for this is to overpower any random magnetic fields in the locality of the particle. Then other uniform time-dependent fields in the x and/or y directions are applied to act as controls. Hence the dynamics of the spin-$\frac{1}{2}$ system has the form

$$i\frac{d}{dt}\Psi(t) = \frac{\gamma}{2}(\sigma_z B_0 + \sigma_x B_x(t) + \sigma_y B_y(t))\Psi(t) \tag{1.5}$$

By change of variable, we have the control system of simple form

$$i\frac{d}{dt}\Psi(t) = \frac{1}{2}(\sigma_z + \sigma_x \epsilon_x(t) + \sigma_y \epsilon_y(t))\Psi(t) \tag{1.6}$$

It is obvious that the spin-$\frac{1}{2}$ system can be controlled by the inputs $\epsilon_x(t)$ and/or $\epsilon_y(t)$.

The second example of the quantum system is a model to describe the vibrating dynamics of diatomic molecules, which is in an infinite dimensional state space. It appears in all problems involving quantized oscillations, such as in molecular and crystalline vibrations. The Hamiltonian $\mathcal{H}_0$ on state space $X = L^2(\mathbb{R})$ is given by

$$\mathcal{H}_0 = -\frac{h^2}{2m}\frac{d^2}{dr^2} + U(r) \tag{1.7}$$

where h is the Planck's constant, with the Morse potential $U(r)$, which represents the potential energy of a diatomic molecule,

$$U(r) = U_0(1 - e^{-a(r-r_e)})^2 - U_0 \tag{1.8}$$

where r is the distance between the atoms, r_e is the equilibrium bond distance, U_0 is the well depth (defined relative to the dissociated atoms), and a determines the 'width' of the potential. The spectrum of the Hamiltonian operator contains a set of discrete spectrum as well as continuum spectrum, See Figure 1.1. Eigenvalues in the spectrum are called energy levels in quantum mechanics. The discrete energy levels correspond to bound states of the molecular oscillation while the continuous energies correspond to unbounded motion of the diatomic molecules.

Controllability of finite dimensional quantum system where H_0 and H_1 are Hermitian matrix are studied through the method proposed in [9], [67] based on Lie Brackets. However, this characterization does not provide ways to design the control law. In control theory, There are two types of technique to design the control – open-loop control and feedback control. Open loop control can be formulated as a cost functional to be minimized, see in [49], [63]. Using feedback strategy to generate trajectories and open loop control is another way. Some of the references are [14], [59], [48], [3].

For the infinite dimensional control problem of the Schrôdinger equation, there are increasing many literature in the past two decades. Some of references are [55], [2],[30].

The first problem studied in the thesis is the optimal bilinear control of the Schrödinger equation in infinite dimension. The quantum system is prepared at an initial state $\Psi(0, x)$, the control problem is to design a control law to drive the state vector $\Psi(t, x)$ to an orbit of the uncontrolled dynamics

$$i\,\frac{d}{dt}\mathcal{O}(t) = \mathcal{H}_0\mathcal{O}(t), \tag{1.9}$$

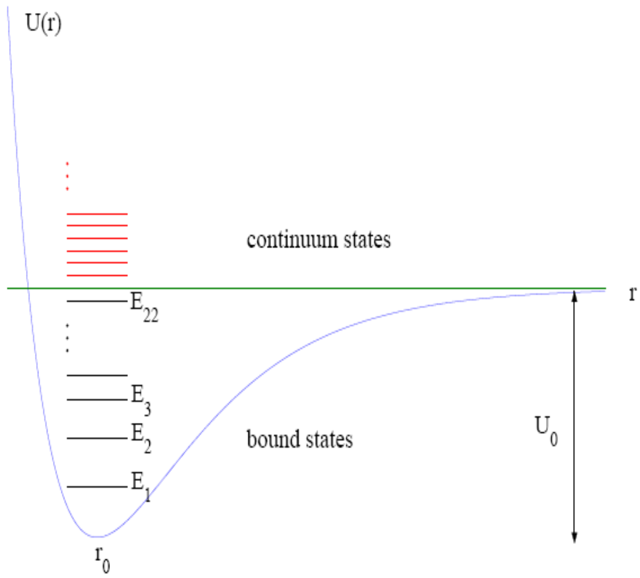

Figure 1.1: The energy level for oscillator operator with the Morse potential

Similar to the method proposed in [48],[3], we apply a Lyapunov-based approach to find the decaying rate of the orbit tracking functional $V(\Psi, \mathcal{O})$. Based on the functional V, we develop a nonlinear feedback law with switching term to achieve the orbit tracking. We tested the feasibility of the proposed feedback law through numerical simulations, which turns out that the performance of the nonlinear feedback law significantly exceeds the performance of the standard feedback law by incorporating the switching control term. To further improve the orbit tracking performance of the feedback law, we studied and applied the receding horizon synthesis.

In reality, the state of a quantum system is inherently nondeterministic in nature due to the interaction with external environment. In the microworld each experiment results in interaction with the system. No quantum measurement can give full information on the state of a quantum system. Hence the measurement and feedback in quantum systems lead to much more complicated model and dynamics than the simple Schrödinger equation. One of the examples of quantum measurement is the Stern-Gerlach experiment. (Figure 1.2). In the experiment, an ensemble of spin-$\frac{1}{2}$ particles pass through an inhomogeneous magnetic field. The position of a particle collected on the plate indicates the force acting on the particle. The Stern-Gerlach experiment has shown that only two locations on the plate are possible for the particles, instead of distributed continuously as classical theory indicates. These two locations correspond to spin up and spin down. This suggests that the interaction of a quantum system with its environment makes its evolution nonunitary and induces relaxation to some equilibrium state.

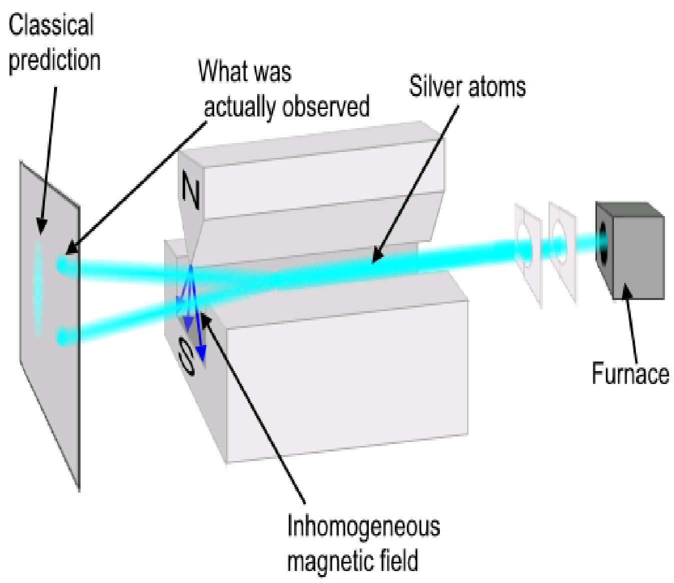

Figure 1.2: Demonstration for the Stern-Gerlach experiment

An open quantum system is used to denote a quantum system with measurement. Let ρ_t be the density matrix, which can be used to measure the outcomes of observables, such as position, spin in quantum system. In particular, $\rho_t = \Psi_t \Psi_t^T$ for some wave function Ψ_t if ρ_t is a pure state. Under continuous measurement, the evolution of ρ_t, which describes the evolution of the open quantum system, satisfies the Lindbald-Kossakowski equation,

$$\frac{d\rho}{dt} = -i[H, \rho] + \sum_{k=1}^{N} L_k \rho_t L_k^* - \frac{1}{2}\rho_t L_k^* L - \frac{1}{2} L_k^* L_k \rho_t \tag{1.10}$$

where H is the Hamiltonian, and L_k is the Lindblad operator, which describes the coupling effect of the environment on the quantum system in Born-Markov approximation. Equation (1.10) is also called the quantum master equation. And the Lindblad part $\Gamma\rho_t = \sum_{k=1}^{N} L_k \rho_t L_k^* - \frac{1}{2}\rho_t L_k^* L - \frac{1}{2} L_k^* L_k \rho_t$ is called the dissipation part in quantum chemistry literature. Given ρ_t, the observation process $y(t)$ can be measured by

$$y(t) = \sum_{k=1}^{N} tr(\rho_t L_k^* L_k) \tag{1.11}$$

It is a scalar quantity which can be measured in experiment.

Now let us move on to a prototype of open quantum system: Λ-systems, which typically describe coherent population trapping when a laser irradiates an $(N+1)$ energy level system. See Figure 1.3. The system is composed of N ground state $|g_k\rangle$ and an excited state $|e\rangle$. Here the notation $|\Psi\rangle$, which is standard in quantum physics literature, denotes a (wave) vector in the Hilbert space. The objective is to estimate the quantum state by measuring the number of photons per time unit spontaneously emitted from the excited state $|e\rangle$, in other words, the number of clicks (jumps) per time-unit. The density matrix ρ satisfies the quantum master equation with

$$H = \sum_{k=1}^{N} \delta_k \, |g_k\rangle\langle g_k| + \Omega_k \, |g_k\rangle\langle e| + \Omega_k^* \, |e\rangle\langle g_k| \tag{1.12}$$

where $\delta_k \in \mathbb{C}$ is the detuning factor of Quasi resonant laser transition from state $|g_k\rangle$ to state $|e\rangle$; Ω_k is the Rabi pulsations of the transition. Here the notation $|g_k\rangle\langle e|$ stands for the outer product, $|g_k\rangle\langle e| = |g_k\rangle|e\rangle^T$ when both states are finite dimensional vectors. The Lindblad operator L_k corresponding to the spontaneous emission from the state $|e\rangle$ towards $|g_k\rangle$ are given as follows

$$L_k = \sqrt{\Gamma_k} \, |g_k\rangle\langle e| \tag{1.13}$$

where Γ_k is the spontaneous emission rate from $|e\rangle$ to $|g_k\rangle$.

In the above setting, the Rabi Pulsation Ω_k can be used as the control input to control the coherent source of photons. This process is known as laser cooling for Λ-systems. Some reference can be found in [69] [65].

As quantum systems are indeterministic, it is natural to use stochastic theory to model the quantum state with random effects. Following the quantum filtering theory by Belavkin [4] in 1990s, a quantum state subject to continuous measurement can be modeled by a classical stochastic differential equation, called quantum filtering equation. After that, techniques in stochastic control theory can be applied to study the quantum control problem with measurement, [23] [24] [47]. Let ρ_t be the density matrix, the quantum stochastic

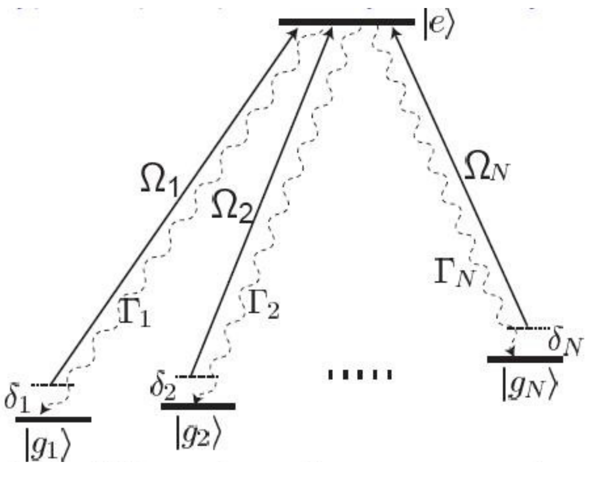

Figure 1.3: Diagram of Λ-systems

differential equation (QSDE) for ρ_t under measurement of homodyn detection follows

$$d\rho_t = (-i[H, \rho_t] + L\rho_t L^* - \frac{1}{2}\rho_t L^* L - \frac{1}{2}L^* L\rho_t)dt + (L\rho_t + \rho_t L^* - Tr[\rho_t(L + L^*)]\rho_t)dW_t \tag{1.14}$$

where $dW_t = dY_t - Tr((L^* + L)\rho_t)dt$ is the innovation process to describe the randomness in the measurement of quantum state. W_t is the Wiener process, Y_t is the measurement process. Comparing to equation (1.10), we see here the number of Lindblad operator is 1 and the stochastic term is included in (1.14).

For a quantum control problem, typically the Hamiltonian H is in the form of

$$H = H_0 + u_t V$$

where H_0 is the internal Hamiltonian and the system is controlled by an external field V through control input u_t. To have the stochastic stability of the quantum system at a ground state is an important problem in fields, such as quantum information and quantum computing. Some applications are quantum state preparation, laser cooling of atoms and molecules.

In the thesis, we study the problem of global stabilization of a quantum spin system under the noisy environment and continuous measurement via feedback control. We propose and implemente a new nonlinear feedback control law with switching term to globally stabilize the quantum spin system at an equilibrium state. A positive definite preserving scheme is analyzed and implemented for the numerical simulation.

1.2 Control of Tumor Growth

A lot of control problems have the similar mechanism as the orbit tracking control problem of the Schrödinger equation, that is, to control the state of a system to a stable state corresponding to the uncontrolled system. Hence we believe the switching mechanism can be applied to a wide general class of control systems and feedback synthesis based on the Lyapunov stability. By using this principle, we study the control problem of a tumor growth model. Its aim is to reduce the tumor cell population in the environment.

As cancer is one of the main causes of mortality in the world, to find a treatment to kill or suppress the tumor growth is one of the urgent tasks in medicine. In the past few years, lots of mathematical models have been proposed to describe the tumor growth, see [13] [60]. And several papers have been published on the optimal tumor treatment planning strategies, based on mathematical models and control theory, see [56] [64]. They help to provide insights and motivation for practically designing certain drugs and strategies for tumor treatment.

In the thesis, we study the control problem of tumor growth model in which tumor cell growth are represented by a reaction-diffusion-convection equation. Let $u(t,x)$ represent the local density of tumor cells at time $t \in [0,\infty]$ and at location $x \in \Omega \subset \mathbb{R}^3$. The dynamics of tumor cell subject to drug dose treatment can be modeled as

$$\frac{\partial u}{\partial t} + \nabla \cdot (vu) = \nabla \cdot (D\nabla u) + \lambda(u,c) - \mu(u,c) - \epsilon(t)\chi_\omega(u,c) \tag{1.15}$$

here c denotes concentrations of the chemical species, such as oxygen, glucose, which provide nutrients for tumor cell. v denote the velocity of cell movement due to proliferation, D is the diffusion constant. $\lambda(u,c)$, $\mu(u,c)$ are the internal chemical dependent cell production and death before treatment. The tumor treatment is achieved by applying the drug dose effect $\chi_\omega(u,c)$ on a localized region ω at rate $\epsilon(t)$. The control problem is to find a time dependent control $\epsilon(t) \in L^2(0,\infty)$ which drives $\|u(t)\|_\infty$ close to 0 as t goes to infinity.

We employ the variational approach to design a nonlinear feedback law with switching term to suppress the tumor growth. Numerical simulation is performed to demonstrate the effectiveness of the feedback law to control the tumor growth to some equilibrium.

1.3 Time Optimal Control

Due to their practical relevance and inherent structural difficulties, time optimal control problems have been received considerable amount of attention for decades. This type of problem arises in wide fields, such as engineering and material sciences. To name some of these problems in application, they are time optimal control on the Kepler equation for the orbital transfer of satellite [12] [11], time optimal control on quantum spin system [35] [73], and time optimal control of flexible space structures [25].

The time optimal control problem is to choose a control in such a way that a dynamical system reaches a target state or manifold in minimum time. Without control constraints, such problems may not have a solution. In the presence of control constraints, the optimal control will typically be of bang-bang form. The problem can be stated as

$$\min \quad \tau = \int_0^\tau 1\,dt \tag{1.16}$$

$$\text{subject to } \frac{dx(t)}{dt} = f(u(t), x(t)), \quad t \in [0, \tau]; \tag{1.17}$$

$$x(0) = x_0; \quad \Phi(x(\tau)) = 0 \tag{1.18}$$

$$\text{with} \quad |u(t)| \leq \gamma \tag{1.19}$$

By Pontryagin's maximum principle, the necessary optimality system for time optimal control problems contains a multivalued operation which impedes the use of fast numerical methods. Traditional approaches for solving time optimal problems are mainly grouped into direct and indirect methods. Indirect methods are based on multiple shooting techniques [34] to solve the two point boundary value problem. Equipped with a good initial guess for all unknowns, particularly the number and location of the switchings, the shooting method is reported to converge fast and to generate very accurate solutions, for example, see [43]. Direct methods, on the other hand, consider time optimal problems as genuine nonlinear programming problems. They are used in several variants, which frequently involve reparametrization of the controls as the unknowns, see [45] [33]. Much of the literature for time optimal control problem up to the late sixties is covered in [26]. Many recent results can be found in [15] [10] [44]. Time optimal control for infinite dimensional systems is considered in [17], for instance.

In the thesis, one of our objectives is to develop an accurate, efficient and robust numerical method to solve the time optimal control problem for linear and bilinear systems.

Our method is based on a regularization of time optimal control problem and the semi-smooth Newton method. Instead of minimizing the minimum time τ directly as in (1.16), we minimize the cost functional

$$\min_{\tau \geq 0} \int_0^\tau (1 + \frac{\varepsilon}{2}\,|u(s)|^2)\,ds \tag{1.20}$$

for some $\varepsilon > 0$. It is obvious that the cost functional tends to the minimum time τ as $\varepsilon \to 0$. To validate the wellposeness of our approach, we prove that the solution of the regularized problem will converge to the solution of original time optimal control problem asymptotically as the regularization parameter ε tends to 0. In particular monotonic structure of the solutions with respect to ε is shown.

To solve the regularized problem, necessary optimality system is formulated based on Lagrange multiplier theory. Then we apply the semi-smooth Newton method to solve the regularized optimality system. It turns out the method is wellposed and locally superlinearly convergent. By integrating the state and costate and variation of them backwards/forwards in the regularized optimality system, the optimality system is further reduced to a nonlinear equation by semismooth Newton formulation. The Jacobian of the reduced equation is computed for the Newton update of several shooting parameters. The initialization of the Newton method is achieved by solving a related minimum norm problem, which gives a reasonable initial guess of the shooting parameters. Continuation method is also applied to globalize the semi-smooth Newton method. The continuation parameters can be set to be the time horizon, the target state, or bounds of control, etc.

We also study a counterpart of time optimal control problem, namely the minimum effort problem. While the time optimal control problem finds the minimum time to reach the target, the minimum effort problem addresses a question of how large control needs to be so that the target is achieved at a given terminal time T. The problem can be stated as

$$\min \quad \sum_{j=1}^{m} \frac{1}{2}\,|\gamma_j|^2 \tag{1.21}$$

subject to

$$\begin{aligned} &\frac{d}{dt}x(t) = f(u(t), x(t)), \quad x(0) = x_0, \;\; \Phi(x(T)) = 0 \\ &\text{with} \quad |u_j(t)| \leq \gamma_j \end{aligned} \tag{1.22}$$

where the control $u = \{u_j\}$ for $j = 1, \ldots, m$. Similar to the time optimal control problem, the control law for the minimum effort problem is also bang-bang. Hence similar regularization process and semi-smooth Newton method is applied to solve the associate optimality system for the minimum effort problem.

To demonstrate the effectiveness of our proposed method, a lot of examples, such as harmonic oscillator, have been tested. Then we formulate the time optimal control problem for quantum spin-$\frac{1}{2}$ system and show the time optimal solution for spin-$\frac{1}{2}$ system to a ground state. Numerical results of time optimal control problem for infinite dimensional systems is also presented in the thesis. For example, the heat equation through boundary control is studied.

1.4 Thesis Organization

The thesis is organized as follows:

In Chapter 2, we start with an introduction of quantum mechanics, and formulate the orbit tracking problem for the Schrödinger equation. The nonlinear feedback law with switching term is developed. Numerical method is described and implemented to demonstrate the feasibility of the proposed feedback synthesis.

In Chapter 3, the receding horizon control synthesis is applied to improve the performance of the feedback law studied in Chapter 2.

In Chapter 4, we formulate the control problem for a tumor growth model. Feedback control law based on Lyapunov techniques is developed. A 2-D example is studied for the numerical simulation.

In Chapter 5, we start from studying the quantum probability theory and quantum filtering theory to derive the quantum filtering equation for quantum systems with continuous measurement. The problem of global stabilization of a quantum spin system under the noisy environment and continuous measurement via feedback control is studied.

In Chapter 6, time optimal and minimum effort control problem for linear and bilinear system are studied. Regularized problems are formulated and the semismooth Newton method is applied to solve the regularized optimality system. The effectiveness of our approach is demonstrated by several examples. Time optimal control problems of quantum spin-$\frac{1}{2}$ system and the heat equation through boundary control are presented.

Finally, Chapter 7 contains some concluding remarks and indicates some directions for future work.

Chapter 2

Feedback Control of the Schrödinger Equation

In this chapter, we study the orbit tracking problem for the Schrödinger equation via feedback control. A nonlinear feedback law with switching term is developed and the asymptotic properties of the feedback laws are analyzed by the LaSalle-type invariance principle.

2.1 Introduction to Quantum Mechanics

Quantum mechanics is a fundamental branch of physics to study the behaviors of microscopic particles. In this section, We present some of the main notions of quantum mechanics and formulate the basic principles using mathematical language. For a complete description of quantum mechanics theory, we refer to [68] [62] [21].

In quantum mechanics, every physical system is associated with a Hilbert Space $\mathscr{H}$. Central in quantum mechanics are the notions of observables X, which consists of all self-adjoint operators on $\mathscr{H}$. Observables represent physical quantities which describe the status of physical systems. Some examples of observables are position, momentum, spin, etc. Any observable X, being a self-adjoint operator, has the spectral decomposition,

$$X = \sum_{a \in spec(X)} a P_a \tag{2.1}$$

where a are its eigenvalues and P_a are the projection operators of the eigenvectors.

A state is used to measure the quantities associated with observable. On a finite dimensional Hilbert space $\mathscr{H}$, it is represented by a density matrix ρ, which is a self-adjoint operator on H that is positive $\rho \geq 0$ and normalized $Tr(\rho) = 1$. That is, it belongs to the set

$$S = \{\rho \in \mathcal{C}^{N\times N} : \rho^* = \rho, \rho \geq 0, Tr(\rho) = 1\} \tag{2.2}$$

Pure states are projection operators onto one-dimensional subspace of $\mathscr{H}$. All the other states are called mixed states. It can be proved that a state ρ is a pure state if and only if $Tr(\rho^2) = 1$.

It's easy to show that the set S of density matrices is convex. The extremal points are uniquely specified by a unit vector $\Psi \in H$, such that $Tr(\rho X) =< \Psi, X\Psi >$. The unit vector Ψ in $\mathscr{H}$ is called a pure state vector, which corresponds to a pure state.

A measurement is a physical procedure or experiment that produces numerical results related to observables. In any given measurement, the allowable results take values in the spectrum of a chosen observable X. The probability of the event P_a, i.e., the observable X takes the values a in the state ρ, is equal to $Tr(\rho P_a)$. In particular, the expectation of an observable X is given by $Tr(\rho X)$.

The variance of the observable X in the state ρ, which measures the mean deviation of X from its expectation, is defined by

$$var_\rho(X) = Tr(\rho X^2) - (Tr(\rho X))^2$$

For any pure state ρ and observables X, Y, we have the following inequality which is well known as Heisenberg uncertainty principle in quantum mechanics, see in [68].

$$var_\rho(X)var_\rho(Y) \geq \frac{1}{4}| < \rho, i[X, Y]\rho > |^2 \tag{2.3}$$

where the Lie bracket is defined as $[X, Y] = XY - YX$.

Heisenberg's uncertainty principle provides a quantitative expression of the fact that even in a pure state, non-commuting observables cannot be measured simultaneously. In other words, even pure states do not give deterministic measurement outcomes for all observables. This shows a fundamental difference between the process of measurement in classical mechanics and in quantum mechanics.

So far we have considered a physical system at certain time, we shall now take into account the time evolution of the state ρ or the state vector Ψ corresponds to pure state.

If U is a unitary operator, ρ is a state and P_a is an event of observable X, then $U\rho U^*$ is also a state, U^*P_aU is an event and $Tr(U\rho U^*P_a) = Tr(\rho U^*P_aU)$. Hence we can describe the evolution of a quantum system in a unitary fashion: Let U_t be a unitary operator such that $U_t = e^{-itH}$, where H is called the stone generator of the group $\{U_t|t \in \mathbb{R}\}$. If ρ is the state at time 0, the state ρ_t at time t is given by $\rho_t = U_t\rho U_t^*$. This can be equivalently described by the differential equation

$$\frac{d\rho_t}{dt} = -i[H, \rho_t], \quad \rho_0 = \rho \tag{2.4}$$

If ρ is a pure state, which corresponds to a state vector Ψ, then the evolution of the state vector $\Psi_t = U_t\Psi$ satisfies the famous time-dependent Schrödinger equation

$$i\frac{d\Psi_t}{dt} = H\Psi_t, \quad \Psi_0 = \Psi \tag{2.5}$$

where now H is known as the Hamiltonian for the dynamics. The above derivation is known as the Schrodinger picture.

Equivalently, we can describe the dynamics of an observable X at time t, $X_t = U_t^*XU_t$,

$$\frac{dX_t}{dt} = i[H, X_t], \quad X_0 = X \tag{2.6}$$

this is called the Heisenberg equation for the observables. The two pictures are essentially equivalent as $Tr(\rho X_t) = Tr(\rho_t X)$ for any observable X.

Let the state vector Ψ be an eigenvector of the Hamiltonian H, that is

$$H\Psi = \lambda\Psi$$

In physics literature, the eigenvectors of H are called bound state, the corresponding eigenvalues are called energy levels and usually denoted by E.

Now we present some examples of quantum systems. The simplest case is the motion of free quantum particle. Let the Hilbert space $\mathscr{H} = L^2(\mathbb{R})$, the Hamiltonian of a free quantum particle with one degree freedom is given by

$$H_0 = -\frac{h^2}{2m}\frac{d^2}{dx^2} \tag{2.7}$$

which is a self-adjoint operator. Here m is the mass and h is the Planck constant.

Another example is the quantum harmonic oscillator, which appears in all problems involving quantized oscillations, such as molecular and crystalline vibrations. The Hamiltonian H on $\mathscr{H} = L^2(\mathbb{R})$ given by

$$H = -\frac{h^2}{2m}\frac{d^2}{dx^2} + \frac{m\omega^2 x^2}{2} \tag{2.8}$$

We set the mass $m = 1$ and define the following operators

$$a = \frac{1}{\sqrt{2\omega h}}(\omega x + i\frac{d}{dx}), \quad a^* = \frac{1}{\sqrt{2\omega h}}(\omega x - i\frac{d}{dx}) \tag{2.9}$$

It can be showed that

$$a^*\Psi_n = \sqrt{n+1}\Psi_{n+1}, \quad a\Psi_n = \sqrt{n}\Psi_{n-1} \tag{2.10}$$

The interpretation is that the operator a^* adds one quantum to the state Ψ_n, hence is called a creation operator. And the operator a destroys one quantum in the state Ψ_n, hence is called an annihilation operator.

The eigen-pairs $(\lambda_k, \Psi_k)_{k=0}^{\infty}$ of the harmonic oscillator H are given by

$$\lambda_k = h\omega(k + \frac{1}{2}), \quad \Psi_n(x) = \hat{c}H_n(\sqrt{\frac{m\omega}{h}}x)e^{-\frac{m\omega}{mh}x^2}$$

where H_k is the Hermite polynomial of degree k and $\hat{c}$ is a normalizing factor. Hence it can be seen that the energy level of the harmonic oscillator H are equally distributed by $h\omega$. The vector Ψ_0 is called the ground state.

In general, we present the Hamiltonian of the Schrodinger equation to describe the dynamics of a quantum particle in $\mathbb{R}^n$ moving in a potential field. To simplify the notation, we set $h = 1$ and $m = \frac{1}{2}$, and use $x = (x_1, \ldots, x_n)$ for the Cartesian coordinates on $\mathbb{R}^n$. On Hilbert space $\mathscr{H} = L^2(\mathbb{R}^n)$, the Hamiltonian is given by

$$H = -\Delta + V(x)$$

where

$$H_0 = -\Delta = -(\frac{\partial^2}{\partial x_1^2} + \ldots + \frac{\partial^2}{\partial x_n^2})$$

and $V(x)$ is a real valued measurable function on $\mathbb{R}^n$, which is called the potential energy operator.

2.2 Formulation of the Problem

Consider a quantum system with internal Hamiltonian $\mathcal{H}_0$ prepared in the initial state $\Psi_0(x)$, where x denotes the relevant spatial coordinate. The state $\Psi(x,t)$ satisfies the time-dependent Schrödinger equation (we set $h = 1$). In the presence of an external interaction taken as an electric field modeled by a coupling operator with amplitude $\epsilon(t) \in \mathbb{R}$ and a time independent dipole moment operator μ results in the controlled Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \epsilon(t)\mu$ and the following dynamical system:

$$i\frac{\partial}{\partial t}\Psi(x,t) = (\mathcal{H}_0 + \epsilon(t)\mu)\Psi(x,t), \quad \Psi(x,0) = \Psi_0(x). \tag{2.11}$$

where $\mathcal{H}_0$ is a positive, closed, self-adjoint operator in the Hilbert space H, $\mu \in \mathcal{L}(H)$ is a bounded self-adjoint linear operator, and $\epsilon \in L^1(0,\infty)$ is the control input.

By setting $\Psi(x,t) = \Psi_1(x,t) + i\,\Psi_2(x,t)$ and $\Psi = (\Psi_1, \Psi_2) \in H \times H$, and let $X = H \times H$ be the complexified Hilbert space corresponding to H, the inner product of X is defined by

$$(\Phi, \Psi)_X = (\Phi_1, \Psi_1)_H + (\Phi_2, \Psi_2)_H + i\big((\Phi_2, \Psi_1)_H - (\Phi_1, \Psi_2)_H\big),$$

where $\Phi = (\Phi_1, \Phi_2)$, $\Psi = (\Psi_1, \Psi_2)$. Throughout we normalize the initial state by $|\Psi_0|_X = 1$.

By separating the corresponding real and imaginary parts, equation (2.11) can equivalently be written as

$$\frac{\partial}{\partial t}\Psi_1(x,t) = (\mathcal{H}_0 + \epsilon(t)\mu)\Psi_2(x,t) \tag{2.12}$$

$$\frac{\partial}{\partial t}\Psi_2(x,t) = -(\mathcal{H}_0 + \epsilon(t)\mu)\Psi_1(x,t) \quad \text{for} \quad (x,t) \in \Omega \times (0,T] \tag{2.13}$$

Here $T > 0$ and $\Omega = \mathbb{R}^n$ or Ω is a bounded subset of $\mathbb{R}^n$. We define the closed linear operator A_0 in $X = H \times H$ by

$$A_0 = \begin{pmatrix} 0 & \mathcal{H}_0 \\ -\mathcal{H}_0 & 0 \end{pmatrix}$$

with $dom(A_0) = dom(\mathcal{H}_0) \times dom(\mathcal{H}_0)$. We note that

$$|(\Psi_1, \Psi_2)|_{H\times H} = |\Psi|_X, \text{ and } (\Phi, \Psi)_{H\times H} = Re(\Phi, \Psi)_X = \Phi_1\Psi_1 + \Phi_2\Psi_2,$$

Lemma 2.2.1 *the operator A_0 is skew-adjoint, i.e.,*

$$(A_0\Psi, \hat{\Psi})_{H\times H} = -(A_0\hat{\Psi}, \Psi)_{H\times H} \textit{ for all } \Psi, \hat{\Psi} \in dom\,(A_0).$$

Proof:

$$
\begin{aligned}
(A_0\Psi, \hat{\Psi})_{H\times H} &= (\begin{pmatrix} 0 & \mathcal{H}_0 \\ -\mathcal{H}_0 & 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix}, \begin{pmatrix} \hat{\Psi}_1 \\ \hat{\Psi}_2 \end{pmatrix})_{H\times H} \\
&= (\begin{pmatrix} \mathcal{H}_0\Psi_2 \\ -\mathcal{H}_0\Psi_1 \end{pmatrix}, \begin{pmatrix} \hat{\Psi}_1 \\ \hat{\Psi}_2 \end{pmatrix}) = \mathcal{H}_0\Psi_2\hat{\Psi}_1 - \mathcal{H}_0\Psi_1\hat{\Psi}_2
\end{aligned}
$$

Similarly, we have $(A_0\hat{\Psi}, \Psi)_{H\times H} = \mathcal{H}_0\hat{\Psi}_2\Psi_1 - \mathcal{H}_0\hat{\Psi}_1\Psi_2 = \mathcal{H}_0\Psi_1\hat{\Psi}_2 - \mathcal{H}_0\Psi_2\hat{\Psi}_1$, since $\mathcal{H}_0$ is self-adjoint. □

Hence for any skew-adjoint operator A_0, we have $(A_0\Psi, \hat{\Psi})_{H\times H} = 0$. Associate to the self-adjoint operator $\mu \in \mathcal{L}(H)$, we can also define

$$
B = \begin{pmatrix} 0 & \mu \\ -\mu & 0 \end{pmatrix}
$$

which is easily to seen to be a skew-adjoint operator. Then system (2.12) (2.13) can be written in a bilinear form,

$$
\frac{d}{dt}\Psi(t,x) = A_0\Psi(t,x) + \epsilon(t)B\Psi(t,x) \tag{2.14}
$$

It can be showed that the controlled Schrödinger equation is norm-preserving. That is, $|\Psi(t)|_X = 1$ for all $t \geq 0$ with the normalized initial state $|\Psi_0| = 1$.

Lemma 2.2.2 $|\Psi(t)|_X = 1$ *for all* $t \geq 0$*, given* $|\Psi_0| = 1$*.*

Proof: Consider the following

$$
\frac{1}{2}\frac{d}{dt}|\Psi|_X^2 = (\Psi, \frac{d\Psi}{dt})_X = (\Psi, A_0\Psi + \epsilon B\Psi) = 0
$$

since A_0 and B are skew-adjoint operator. Hence $|\Psi(t)|_X = |\Psi_0|_X = 1$. □

In the thesis, we consider the control problem of driving the state $\Psi(t)$ of (2.11) to an orbit $\mathcal{O}(t)$ of the uncontrolled dynamics

$$
i\frac{d}{dt}\mathcal{O}(t) = \mathcal{H}_0\mathcal{O}(t), \tag{2.15}
$$

specifically to the one that corresponds to an eigen-state or the manifold spanned by finite many eigen-states. An element $\psi \in dom\,(\mathcal{H}_0)$ is an eigen-state of $\mathcal{H}_0$ if $\mathcal{H}_0\psi = \lambda\,\psi$ for the eigenvalue $\lambda > 0$. Then, the corresponding orbit is given by

$$\mathcal{O}(t) = e^{-i(\lambda t-\theta)}\psi, \tag{2.16}$$

where $\theta \in [0, 2\pi)$ is the phase factor. We have $|\mathcal{O}(t)|_X = 1$ if ψ is normalized as $|\psi|_X = 1$. In general,

$$\mathcal{O}(t) = \sum_{k=1}^{N} A_k e^{-i(\lambda_k t-\theta_k)}\psi_k, \tag{2.17}$$

where $\{(\lambda_k, \psi_k)\}_{k=1}^N$ are the first N eigen-pairs of $\mathcal{H}_0$ and $\sum_{k=1}^N A_k^2 = 1$.

Here we consider the discrete spectrum case: i.e. assume $\mathcal{H}_0$ only has discrete eigenvalues $\{\lambda_k\}$, the family of eigenfunctions $\{\psi_k\}_{k=1}^\infty$ forms an orthonormal basis of X and that $\{\lambda_k\}$ are arranged in increasing order. For example, Let $H = L^2[0, \pi]$, $\mathcal{H}_0\Psi = \frac{d^2\Psi}{dx^2}$ with

$$dom(\mathcal{H}_0) = \{\psi \in L^2(0, \pi) : \frac{d\psi}{dx}, \frac{d^2\psi}{dx^2} \in L^2(0, \pi) \text{ and } \psi(0) = \psi(\pi) = 0\}$$

It can be showed that the eigenvalue and eigenfunctions of the operator $\mathcal{H}_0$ are given by $\lambda_k = -k^2$, $\Psi_k = \sqrt{\frac{2}{\pi}} sinkx$, $k = 1, 2, \ldots$.

Our objective is to construct a time dependent control rule $\epsilon(t)$ which drives the quantum system from initial state $\Psi_0(x)$ to an orbit (2.16). To fulfill this, we employ a variational approach based on the Lyapunov functional

$$V(t) = V(\Psi(t), \mathcal{O}(t)) = \frac{1}{2}\,|\Psi(t) - \mathcal{O}(t)|_X^2. \tag{2.18}$$

Notice that if $V(t) \to 0$ as $t \to \infty$ for a controlled state Ψ of (2.11), then $\Psi(t)$ achieves the tracking of the target orbit $\mathcal{O}(t)$ asymptotically. Variational approaches were previously discussed in [3] [48] [30], for example.

There is another functional

$$V_2(t) = \frac{1}{2}(1 - |(\mathcal{O}(t), \Psi(t))_X|^2) \tag{2.19}$$

in [3] [48], which is used for for the manifold tracking, since V_2 is motivated by the fact that $V_2(\Psi, \mathcal{O}) = 0$ if and only if $\Psi = e^{i\theta}\mathcal{O}$ where the phase $\theta \in [0, 2\pi)$ is arbitrary.

We develop a feedback synthesis that achieves the orbit tracking based on the functional V defined by (2.18). By lemma (2.2.2) together with $|\mathcal{O}(t)|_X = 1$, it implies that the functional V can equivalently be expressed as

Lemma 2.2.3

$$V(\Psi(t), \mathcal{O}(t)) = 1 - Re\,(\mathcal{O}(t), \Psi(t))_X. \tag{2.20}$$

Proof:

$$\begin{aligned} V(t) &= \frac{1}{2}((\Psi(t) - \mathcal{O}(t), \Psi(t) - \mathcal{O}(t))_X \\ &= \frac{1}{2}(\Psi(t), \Psi(t))_X - (\Psi(t), \mathcal{O}(t))_X - (\mathcal{O}(t), \Psi(t))_X + (\mathcal{O}(t), \mathcal{O}(t))_X) \\ &= \frac{1}{2}(1 + 1 - 2\mathrm{Re}\,(\mathcal{O}(t), \Psi(t))_X) = 1 - \mathrm{Re}\,(\mathcal{O}(t), \Psi(t))_X. \quad \square \end{aligned}$$

Apply the Lyapunov technique to find the rate of change of $V(\Psi(t), \mathcal{O}(t))$, we have

Proposition 2.2.1

$$\frac{d}{dt}V(\Psi(t), \mathcal{O}(t)) = \epsilon(t)\, Im\,(\mathcal{O}(t), \mu\Psi(t))_X. \tag{2.21}$$

Proof:

$$\frac{d}{dt}\mathrm{Re}\,(\mathcal{O}(t), \Psi(t))_X = \mathrm{Re}\,\big((-i\,\mathcal{H}_0\mathcal{O}(t), \Psi(t))_X + (\mathcal{O}(t), -i(\mathcal{H}_0\Psi(t) + \epsilon(t)\mu\Psi(t))_X\big)$$

$$= \mathrm{Re}\big(i\,\epsilon(t)\,(\mathcal{O}(t), \mu\Psi(t))\big)_X = -\epsilon(t)\,\mathrm{Im}\,(\mathcal{O}(t), \mu\Psi(t))_X,$$

hence

$$\frac{d}{dt}V(\Psi(t), \mathcal{O}(t)) = -\frac{d}{dt}\mathrm{Re}\,(\mathcal{O}(t), \Psi(t))_X = \epsilon(t)\,\mathrm{Im}\,(\mathcal{O}(t), \mu\Psi(t))_X.\square$$

Note that the functional $V(\Psi(t), \mathcal{O}(t))$ is a function with value in $[0, 1]$, and $V(\Psi(t), \mathcal{O}(t)) \to 0$ as $\Psi(t) \to \mathcal{O}(t)$, thus we wish the rate of change of $V(\Psi(t), \mathcal{O}(t))$ to be negative. We propose the nonlinear feedback law

$$\begin{aligned} \epsilon(t) &= -\frac{1}{\alpha}(u(t) + \beta\,\mathrm{sign}(u(t))V(t)^\gamma) = F(\Psi(t), \mathcal{O}(t)), \\ u(t) &= \mathrm{Im}\,(\mathcal{O}(t), \mu\Psi(t))_X, \quad V(t) = V(\Psi(t), \mathcal{O}(t)), \end{aligned} \tag{2.22}$$

for $\alpha > 0,\ \beta \geq 0,\ \gamma \in (0, 1]$. From (2.21), we have

$$\frac{d}{dt}V(\Psi(t), \mathcal{O}(t)) = -\frac{1}{\alpha}\,(|u(t)|^2 + \beta\,|u(t)|V(t)^\gamma). \tag{2.23}$$

So that

$$V(\Psi(t), \mathcal{O}(t)) = V(\Psi(0), \mathcal{O}(0)) - \int_0^t \frac{1}{\alpha}(|u(s)|^2 + \beta|u(s)|V(\Psi(s), \mathcal{O}(s))^\gamma)ds \qquad (2.24)$$

Note that $u(t)$ is linear in $\Psi(t)$ and the second term of the control law (2.22) can switch its sign. The case $\beta = 0$ is a negative feedback law based on the Lyapunov energy equality (2.21) and was analyzed in [30]. It will be shown in Section 2.7 that the performance of the feedback law (2.22) significantly increases by incorporating the switching control term with $\beta > 0$ by numerical evidence.

We believe this switching mechanism can be applied to a wide general class of control systems and feedback synthesis based on the Lyapunov stability. A example is demonstrated for the switching mechanism in Chapter 4 on the control problem of a tumor growth model.

In order to obtain improved tracking capability, we also analyze cases with multiple control potentials of the form

$$\mu(t) = \sum_{j=1}^m \epsilon_j(t)\, \mu_j \qquad (2.25)$$

and the corresponding feedback law

$$\epsilon_j(t) = -\frac{1}{\alpha}(u_j(t) + \beta\, \mathrm{sign}(u_j(t))V(t)^\gamma), \quad u_j(t) = \mathrm{Im}\,(\mathcal{O}(t), \mu_j\Psi(t))_X.$$

Later in section 2.6, we will show that in order to have asymptotic tracking properties by the feedback law (2.22), multiple control potentials need to be taken for some Hamiltonian H_0.

2.3 Well-posedness

In this section, we establish the well-posedness of the feedback law (2.22). That is, there exists a solution $\Psi(t) \in X = H \times H$ for the system

$$\frac{d}{dt}\Psi(t) = A_0\Psi(t) + \epsilon(t)B\Psi(t) \quad \Psi(0) = \Psi_0$$

with the feedback control law

$$\epsilon(t) = -\frac{1}{\alpha}(u(t) + \beta\, \mathrm{sign}(u(t))V(t)^\gamma) = F(\Psi(t), \mathcal{O}(t)),$$

in the form of

$$\Psi(t) = S(t)\Psi_0 + \int_0^t S(t-s)F(\Psi(s), \mathcal{O}(s))B\Psi(s)\,ds \tag{2.26}$$

In section (2.2), we defined the closed linear operator A_0 in $H \times H$ by

$$A_0 = \begin{pmatrix} 0 & \mathcal{H}_0 \\ & \\ -\mathcal{H}_0 & 0 \end{pmatrix}$$

with $dom\,(A_0) = dom\,(\mathcal{H}_0) \times dom\,(\mathcal{H}_0)$, and show A_0 is skew-adjoint in Lemma (2.2.1). Thus by Stone's theorem [54], A_0 generates C_0-group $S(t)$ on X and $|S(t)\Psi_0|_X = |\Psi_0|_X$.

A family of bounded linear operators $X \to X$, $S(t)$, $t > 0$ is called a C_0-semigroup on X (also strongly continuous semigroup) if and only if the following properties hold:

$$S(0) = I,$$

$$S(t)S(s) = S(t+s), t, s \geq 0, \text{ (semigroup property)}$$

$$\lim_{t \to 0^+} |S(t)x - x| = 0 \text{ for all } x \in X \text{ (strong continuity at 0)}$$

Let $S(\cdot)$ be a C_0-semigroup on X. The linear operator A defined by

$$\mathrm{dom}\,A = \{x \in X |\lim_{t \to 0^+} \frac{1}{t}(S(t)x - x) \text{ exists}\},$$

$$Ax = \lim_{t \to 0^+} \frac{1}{t}(S(t)x - x), x \in \mathrm{dom}\,A,$$

is called the infinitesimal generator of $S(\cdot)$.

The function $u \in C([0,T] : X)$ given by

$$u(t) = S(t)x_0 + \int_0^t S(t-s)f(s)\,ds, \quad 0 \leq t \leq T$$

is the mild solution of the cauchy problem

$$\begin{aligned} &\frac{d}{dt}u(t) = Au(t) + f(t), \quad t \geq 0, \\ &u(0) = x_0, \end{aligned} \tag{2.27}$$

on $[0,T]$, where the operator A on X is the infinitesimal generator of a C_0-semigroup $S(\cdot)$ and the function $f \in L^1(0,T : X)$.

Let $V = dom\,(\mathcal{H}_0^{\frac{1}{2}})$ and $X_2 = V \times V$. Then $\mathcal{H}_0 \in \mathcal{L}(V, V^*)$ with $V^* = dom\,(\mathcal{H}_0^{-\frac{1}{2}})$ and V is equipped with

$$|\phi|_V^2 = \langle \mathcal{H}_0\phi, \phi\rangle_{V^* \times V}$$

as norm. The restriction of $S(t)$ to X_2 defines a C_0 group.

Associated to the self-adjoint operator $\mu \in \mathcal{L}(H)$, we define the skew-adjoint operator

$$B = \begin{pmatrix} 0 & \mu \\ & \\ -\mu & 0 \end{pmatrix}$$

Then for $\epsilon \in L^2(0,T)$ there exists a unique mild solution $\Psi(t) \in C(0,T;X)$ to

$$\Psi(t) = S(t)\Psi_0 + \int_0^t S(t-s)\epsilon(s)\, B\Psi(s)\, ds, \quad t \in [0,T], \tag{2.28}$$

and

$$\frac{d}{dt}\Psi = A_0\Psi(t) + \epsilon(t)B\Psi(t) \quad \text{in } (dom\,(A_0))^*, \tag{2.29}$$

where

$$(dom\,(A_0))^* = dom\,(\mathcal{H}_0^{-1}) \times dom\,(\mathcal{H}_0^{-1}),$$

[29], Chapter2, [54], Chapter 4. Equivalently

$$i\frac{d}{dt}\Psi(t) = (\mathcal{H}_0\Psi(t) + \epsilon(t)\mu\Psi(t)) \text{ in } dom(\mathcal{H}_0^{-1})$$

where we identify $\Psi \in X$ as $\Psi = \Psi_1 + i\Psi_2$ by $\Psi = (\Psi_1, \Psi_2) \in H \times H$. Since $\mathcal{O}(t)$ defined by (2.16) and (2.17) satisfy $\mathcal{O}(t) \in C(0,T;dom\,(A_0)) \cap C^1(0,T;X)$ and

$$i\frac{d}{dt}\mathcal{O}(t) = \mathcal{H}_0\mathcal{O}(t) \text{ in } H. \tag{2.30}$$

In (2.22), we propose the feedback law $\epsilon(t) = F(\Psi(t), \mathcal{O}(t))$, thus, we obtain the closed loop system of the form

$$\Psi(t) = S(t)\Psi_0 + \int_0^t S(t-s)F(\Psi(s), \mathcal{O}(s))B\Psi(s)\, ds \tag{2.31}$$

We show that (2.31) has a solution. Let $\mathrm{sign}(u)$ be the maximal monotone function

$$\mathrm{sign}(u) = \begin{cases} [-1,1] & u = 0 \\ & \\ \dfrac{u}{|u|} & |u| > 0, \end{cases}$$

and $\mathrm{sign}_\delta(u)$ be the Yosida approximation of $\mathrm{sign}(u)$ for $\delta > 0$:

$$\mathrm{sign}_\delta(u) = \begin{cases} \dfrac{u}{\delta} & |u| \le \delta \\ \\ \dfrac{u}{|u|} & |u| \ge \delta. \end{cases}$$

Define the operators F_δ by

$$F_\delta(\Psi, \mathcal{O}) = -\frac{1}{\alpha}(u + \beta\, \mathrm{sign}_\delta(u) V^\gamma), \quad u = \mathrm{Im}\,(\mathcal{O}(t), \mu\Psi). \tag{2.32}$$

Assuming that $V \ge c > 0$, then F_δ is Lipschitz continuous with respect to Ψ, and $|F_\delta| \le M$ for all $|\Psi|_X = |\mathcal{O}|_X = 1$. Thus, it can be proved [29],[31] that

$$\Psi(t) = S(t)\Psi_0 + \int_0^t S(t-s) F_\delta(\Psi(s), \mathcal{O}(s)) B\Psi(s)\, ds$$

has a unique solution $\Psi_\delta \in C(0,T;X)$. Moreover by (2.24), we have

$$V_\delta(t) = V(0) - \int_0^t \frac{1}{\alpha}\big(|u_\delta(s)|^2 + \beta\, \mathrm{sign}_\delta(u_\delta)(s) V_\delta(s)^\gamma\big) u_\delta(s)\, ds,$$

where

$$V_\delta(s) = 1 - \mathrm{Re}\,(\Psi_\delta(s), \mathcal{O}(s)), \quad u_\delta(s) = \mathrm{Im}\,(\mathcal{O}(s), \mu\Psi_\delta(s))$$

It follows from [1], Theorem 3.6 that there exists a subsequence δ and $\Psi \in C(0,T;X)$ for which Ψ_δ converges to Ψ in $C(0,T;X)$. Thus $u_\delta(t) \to u(t) = \mathrm{Im}\,(\mathcal{O}(t))(t), \mu\Psi(t))$ strongly in $L^2(0,T;R)$. Since $\mathrm{sign}_\delta(u_\delta(t)) \in L^2(0,T;R)$, by Alaoglu's theorem, there exists a subsequence of δ such that $\mathrm{sign}_\delta(t) \to z(t)$ weakly in $L^2(0,T;R)$. The sign operator is maximal monotone [29] and hence $z(t) = \mathrm{sign}(u(t))$. Since $V_\delta(t) \to V(t)$ in $C(0,T;R)$, $\epsilon_\delta(t) \to \epsilon(t) = u(t) + \mathrm{sign}(u(t))V(t)^\gamma$ weakly in $L^2(0,T;R)$. For all $\phi \in X$

$$(\Psi_\delta(t), \phi) = (S(t)\Psi_0, \phi) + \int_0^t \epsilon_\delta(t)(S(t-s)B\Psi_\delta(s), \phi)\, ds$$

and letting $\delta \to 0^+$ we have

$$(\Psi(t), \phi) = (S(t)\Psi_0, \phi) + \int_0^t \epsilon(t)(S(t-s)B\Psi(s), \phi)\, ds,$$

which implies that Ψ is the mild solution to (2.28) that corresponds to ϵ. Moreover, we have

$$V(t) = V(0) - \int_0^t \frac{1}{\alpha}\,(|u(s)|^2 + \beta\, |u(s)| V(s)^\gamma)\, ds. \tag{2.33}$$

2.4 Optimality

In this section, we show that the proposed feedback synthesis (2.22) is optimal for a given cost functional.

We argue that

$$V(t,\Psi) = 1 - (\mathcal{O}(t),\Psi)_{H\times H}$$

satisfies the Hamilton-Jacobi equation

$$\begin{aligned}&\frac{\partial V}{\partial t} + \min_{\epsilon}[V_\Psi(A_0\Psi + \epsilon B\Psi)]\\ &\quad + \frac{\alpha}{2}|\epsilon + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma|^2 + \frac{1}{\alpha}(\frac{1}{2}|u(t)|^2 + |u(t)|V^\gamma) = 0\end{aligned} \tag{2.34}$$

$$u(t) = \mathrm{Im}\,(\mathcal{O}(t),\mu\Psi)_X = -(\mathcal{O}(t),B\Psi)_{H\times H}$$

where

$$V_\Psi(\Phi) = -(\mathcal{O}(t),\Phi)_{H\times H}.$$

In fact,

$$\begin{aligned}&\frac{\alpha}{2}|\epsilon + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma|^2 + u(t)(\epsilon + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma) + \frac{1}{2\alpha}|u(t)|^2\\ &= \frac{\alpha}{2}|\epsilon + \frac{1}{\alpha}(u(t) + \beta\,\mathrm{sign}(u(t))V^\gamma)|^2,\end{aligned} \tag{2.35}$$

and thus $\epsilon^*(t)$ in (2.22) minimizes

$$\frac{\alpha}{2}|\epsilon + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma|^2 + u(t)(\epsilon + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma) + \frac{1}{2\alpha}|u(t)|^2.$$

This implies

$$\begin{aligned}&\frac{\partial V}{\partial t} + V_\Psi(A_0\Psi + \epsilon^* B\Psi)\\ &\quad + \frac{\alpha}{2}|\epsilon^*(t) + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma|^2 + +u(t)(\frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma|^2 + \frac{1}{2\alpha}|u(t)|^2\\ &= -(A_0\mathcal{O}(t),\Psi)_{H\times H} - (\mathcal{O}(t),A_0\Psi + \epsilon^*(t)B\Psi)_{H\times H}\\ &\quad + \frac{\alpha}{2}|\epsilon^*(t) + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma|^2 + u(t)(\epsilon^*(t) + \frac{\beta}{\alpha}\mathrm{sign}(u(t))V^\gamma)|^2 + \frac{1}{2\alpha}|u(t)|^2 = 0\end{aligned}$$

as desired.

We next show that ϵ^* minimizes the cost functional

$$J(\epsilon) = \int_0^T (\frac{\alpha}{2}|\epsilon(t) + \frac{\beta}{\alpha}\text{sign}(u(t))V(t)^\gamma|^2 + \frac{1}{\alpha}(\frac{1}{2}|u(t)|^2 + \beta\,|u(t)|)\,dt + V(\Psi(t), \mathcal{O}(T),$$

over $\epsilon \in L^2(0,T)$. To this end choose any $\epsilon \in L^2(0,T)$ and let $\Psi(t) \in C(0,T;X)$ be the solution to (2.28)-(2.29). Since $\mathcal{O}(t) \in C^1(0,T;X) \cap C(0,T;dom(A_0)$ we have

$$\frac{d}{dt}V(\mathcal{O}(t), \Psi(t)) = -(A_0\mathcal{O}(t), \Psi(t))_{H\times H} - (\mathcal{O}(t), A_0\Psi(t) + \epsilon(t)B\Psi(t))_{H\times H}.$$

Integrating this over $(0,T)$ and using (2.35) we find

$$V(\Psi(T), \mathcal{O}(T)) + \int_0^T (\frac{\alpha}{2}|\epsilon(t) + \frac{\beta}{\alpha}\,\text{sign}(u(t))V(t)^\gamma|^2 + \frac{1}{\alpha}(\frac{1}{2}|u(t)|^2 + \beta\,|u(t)|V(t)^\gamma)\,dt$$

$$= V(\Psi(0), \mathcal{O}(0)) + \int_0^T \frac{\alpha}{2}\,|\epsilon(t) + \frac{1}{\alpha}(u(t) + \beta\,\text{sign}(u(t))V(t)^\gamma|^2\,dt$$

$$u(t) = (\mathcal{O}(t), B\Psi(t))$$

Hence

$$\epsilon^*(t) = F(\Psi^*(t), \mathcal{O}(t)).$$

where $\Psi^*(t)$ is the trajectory corresponding to $\epsilon^*(t)$ minimizes $J(\epsilon)$ over $L^2(0,T)$.

2.5 Operator Splitting and Numerical Methods

Operator splitting method is often used to solve complex equations where the differential operator in them usually has very complex structure. Due to the complexity, usually there doesn't exist a numerical method which can provide a numerical solution accurate enough, while taking reasonable integration time. The operator splitting method is invented to overcome this. The basic idea behind the operator splitting method is first to decouple the original complex differential operator into a few sub-operators of simpler structure, then solve a sequence of simpler equation corresponding to the sub-operators by some suitable numerical methods. The connections between each sub-system are the initial conditions. The advantages of operator splitting method are that, they can be used to solve equations exactly and the stability and consistency are fulfilled.

There are two types of operator splitting method which are commonly used, see [27]. They are first-order splitting, which is also called sequential splitting and second-order splitting, which is commonly known as Strang splitting [66]. Let us first illustrate the notion of splitting. For simplicity, we consider the cases where the original operator can be written as the sum of two simpler sub-operators.

Consider the following initial value problem

$$\frac{dx(t)}{dt} = Ax + Bx, \quad x(0) = x_0 \tag{2.36}$$

the solution of (2.36) is given by

$$x(t_{n+1}) = e^{\tau(A+B)}x(t_n) \tag{2.37}$$

where $\tau = t_{n+1} - t_n$. The first order splitting method approximated the exact solution (2.37) by

$$x_{n+1} = e^{\tau A}e^{\tau B}x_n \tag{2.38}$$

where x_n approximating $x(t_n)$. It can be shown the splitting error of the method is

$$\rho_n = \frac{1}{\tau}(e^{\tau(A+B)} - e^{\tau A}e^{\tau B})x(t_n) = \frac{1}{2}\tau[A, B]x(t_n) + \mathcal{O}(\tau^2) \tag{2.39}$$

with $[A, B] = AB - BA$ is the Lie bracket. It is why the method is called first order splitting method.

The Strang splitting method is to approximate (2.37) by

$$x_{n+1} = e^{\frac{1}{2}\tau A}e^{\tau B}e^{\frac{1}{2}\tau A}x_n \tag{2.40}$$

Its splitting error is

$$\rho_n = -\frac{1}{24}\tau^2([A, [A, B]] + 2[B, [A, B]])x(t_{n+\frac{1}{2}}) + \mathcal{O}(\tau^4) \tag{2.41}$$

which shows it is a second order method in time integration.

With regard to the stability of operator splitting method, if each sub-operator is stable, then the operator splitting method is also stable.

Since the Hamiltonian of the original system (2.11) is the sum of operators $\mathcal{H}_0$ and $\epsilon(t)\mu$, it is very natural to consider time integration based on the operator splitting method.

For the stepsize $h > 0$ consider the Strang splitting method for (2.14):

$$\frac{\hat{\Psi}_{k+1} - \hat{\Psi}_k}{h} = \epsilon_k\, B\frac{\hat{\Psi}_{k+1} + \hat{\Psi}_k}{2}, \quad \hat{\Psi}_k = S(\frac{h}{2})\Psi_k,$$
$$\Psi_{k+1} = S(\tfrac{h}{2})\hat{\Psi}_{k+1}, \tag{2.42}$$

where

$$\epsilon_k = \frac{1}{h}\int_{kh}^{(k+1)h} \epsilon(s)\, ds.$$

Here $S(\frac{h}{2})$ is the half step time integration of the sub-operator A. For time integration of the controlled Hamiltonian we employ the Crank-Nicolson scheme since it is a norm preserving scheme. In fact, since B is skew adjoint,

$$(\frac{\hat{\Psi}_{k+1} - \hat{\Psi}_k}{h}, \Psi_{k+1} + \hat{\Psi}_k)_X = (\epsilon_k\, B\frac{\hat{\Psi}_{k+1} + \hat{\Psi}_k}{2}, \hat{\Psi}_{k+1} + \hat{\Psi}_k) = 0,$$

and thus $|\hat{\Psi}_{k+1}|_X^2 = |\hat{\Psi}_k|_X^2$.

The following theorem addresses the convergence of the scheme (2.42):

Theorem 2.5.1 *If we define $\Psi_h(t) = \Psi_k$ on $[kh, (k+1)h)$, then*

$$|\Psi_h(t) - \Psi(t)|_X \to 0 \textit{ uniformly in } t \in [0, T]$$

as $h \to 0$, where $\Psi(t)$, $t \geq 0$, is the mild solution satisfying

$$\Psi(t) = S(t)\Psi_0 + \int_0^t S(t-s)\epsilon(s)B\Psi(s)\, ds. \tag{2.43}$$

Proof: Define the one step transition operator

$$\Psi_{k+1} = T_h(t)\Psi_k$$

by

$$T_h(t) = S(\frac{h}{2})(I + \frac{\epsilon_k h}{2}B)(I + \frac{\epsilon_k h}{2}B)^{-1}S(\frac{h}{2})\Psi.$$

Then $|T_h(t)\Psi|_X = |\Psi|_X$, since Crank-Nicolson scheme is norm preserving and $|S(\frac{h}{2})\Psi| = |\Psi|$. Define the difference quotient of $T_h(t)$ by

$$A_h(t)\Psi = \frac{T_h(t)\Psi - \Psi}{h} = S(\frac{h}{2})\frac{J_{h/2}(\epsilon_k B) - I}{h/2}S(\frac{h}{2})\Psi + \frac{S(h)\Psi - \Psi}{h} \tag{2.44}$$

where

$$J_{h/2}(\epsilon_k B) = (I - \frac{\epsilon_k h}{2} B)^{-1}.$$

It follows from the Chernoff theorem [29] that if the consistency

$$|A_h(t)\Psi - (A_0\Psi + \epsilon(t)B\Psi)|_X \to 0 \text{ as } h \to 0^+. \tag{2.45}$$

holds for $\Psi \in dom\,(A)$, then $|\Psi_h(t) - \Psi(t)|_X \to 0$ uniformly in $t \in [0,T]$. In fact, since for $\Psi \in X$

$$\lim_{h\to 0^+} \frac{J_{h/2}(\epsilon_k B) - I}{h/2}\Psi = \epsilon(t)B\Psi$$

and for $\Psi \in dom\,(A)$

$$\lim_{h\to 0^+} \frac{S(h)\Psi - \Psi}{h} = A_0\Psi,$$

it follows from (2.44) that the consistency (2.45) holds for $\Psi \in dom\,(A)$ and $\epsilon \in C(0,T)$. Hence $|\Psi_h(t) - \Psi(t)|_X \to 0$ uniformly in $t \in [0,T]$.

Note that

$$\Psi_{k+1} = S(h)\Psi_k + hS(\frac{h}{2})\epsilon_k J_{h/2}(\epsilon_k B)S(\frac{h}{2})\Psi_k$$

and thus

$$\Psi^m = S(mh)\Psi_0 + \sum_{k=1}^{m} h\,S((m-k)h)S(\frac{h}{2})\epsilon_k B J_{h/2}(\epsilon_k B)S(\frac{h}{2})\Psi_{k-1}.$$

Thus, letting $h \to 0$ in this expression, $\Psi(t) \in C(0,T;X)$ satisfies (2.43). $\square$

Now we describe the discrete scheme for (2.42). Suppose there exists an ϵ_k on $[kh,(k+1)h)$ such that for $\mathcal{O}_{k+1/2} = S(\frac{h}{2})\mathcal{O}_k$,

$$\begin{aligned} &\epsilon_k = F(\Psi_{k+1/2}, \mathcal{O}_{k+1/2}) = \frac{1}{\alpha}(u_{k+1/2} + \beta\,\mathrm{sign}(u_{k+1/2})V_k^{\gamma}), \\ &u_{k+1/2} = (\mathcal{O}_{k+1/2}, B\Psi_{k+1/2}), \quad \Psi_{k+1/2} = \frac{\hat{\Psi}_{k+1} + \hat{\Psi}_k}{2}. \end{aligned} \tag{2.46}$$

Then Ψ_k satisfies the closed loop system

$$\begin{aligned} &\frac{\hat{\Psi}_{k+1} - \hat{\Psi}_k}{h} = \epsilon_k\, B\frac{\hat{\Psi}_{k+1} + \hat{\Psi}_k}{2}, \quad \hat{\Psi}_k = S(\frac{h}{2})\Psi_k, \\ &\epsilon_k = F(\Psi_{k+1/2}, \mathcal{O}_{k+1/2}), \quad \Psi_{k+1} = S(\frac{h}{2})\hat{\Psi}_{k+1}. \end{aligned} \tag{2.47}$$

It can be seen that this is an implicit scheme, as ϵ_k is evaluated at middle point. Since

$$V(S(\frac{h}{2})\hat{\Psi}_{k+1}, S(\frac{h}{2})\mathcal{O}_{k+1/2}) = V(\hat{\Psi}_{k+1}, \mathcal{O}_{k+1/2}),$$

the discrete analog of (2.33)

$$V(\Psi_{k+1}, \mathcal{O}_{k+1}) = V(\Psi_k, \mathcal{O}_k) + \frac{1}{\alpha}(|u_k|^2 + \beta\,|u_k|V(Psi_k, \mathcal{O}_k))^\gamma.$$

holds for the closed loop (2.47).

Now we show that there exists a unique ϵ_k that satisfies (2.46). Let

$$\chi(u) = u + \beta\,\mathrm{sign}(u)$$

Then, it is equivalent to find $\epsilon \in R$ that satisfies

$$\chi^{-1}(\alpha\,\epsilon) = (B\hat{\Psi}(\epsilon), \mathcal{O}_{k+1/2}), \tag{2.48}$$

where $\hat{\Psi}(\epsilon)$ is the solution to

$$\frac{\hat{\Psi} - \hat{\Psi}_k}{h} = \epsilon B \frac{\hat{\Psi} + \hat{\Psi}_k}{2}.$$

hence

$$\hat{\Psi} = (I - \frac{\epsilon B h}{2})^{-1}(I + \frac{\epsilon B h}{2})\hat{\Psi}_k$$

Note that

$$\hat{\Psi} - \hat{\Psi}_k = h\epsilon\, B(I - \frac{h\epsilon}{2}B)^{-1}\hat{\Psi}_k$$

and thus

$$(B\hat{\Psi}(\epsilon), \mathcal{O}_{k+1/2}) = (B\hat{\Psi}_k, \mathcal{O}_{k+1/2}) + h\epsilon(B^2(I - \frac{h\epsilon}{2}B)^{-1}\hat{\Psi}_k, \mathcal{O}_{k+1/2})$$

Since

$$B^2 = \begin{pmatrix} -\mu^2 & 0 \\ & \\ 0 & -\mu^2 \end{pmatrix}$$

one can assume that there exists $c > 0$ for all k

$$(B^2\hat{\Psi}_k, \mathcal{O}_{k+1/2}) \le -c$$

Thus,

$$(B^2(I - \frac{h\epsilon}{2}B)^{-1}\hat{\Psi}_k, \mathcal{O}_{k+1/2}) \le -\frac{c}{2},$$

for $h > 0$ is sufficiently small and hence (2.48) has a unique solution.

2.6 Asymptotic Tracking

Using the Lyapunov technique, we design a nonlinear feedback law (2.22) to make the decay rate of the Lyapunov functional to be negative (2.23). A natural question arises whether the tracked state $\Psi(t)$ will approaches to the orbit $\mathcal{O}(t)$ by the feedback law. In this section, we analyze the asymptotic properties of the controlled system (2.11). We show that under certain conditions, $\Psi(t)$ asymptotically approaches to the orbit $\mathcal{O}(t)$,

$$\lim_{t\to\infty} V(\Psi(t), \mathcal{O}(t)) = 0$$

by the nonlinear feedback law.

Specifically we consider the orbit be of the form

$$\mathcal{O}(t) = e^{-i(\lambda_{k_0} t - \hat{\theta})}\psi_{k_0}$$

for some eigenpair $(\lambda_{k_0}, \psi_{k_0})$ of $\mathcal{H}_0$ and phase $\hat{\theta}$. Assume that

$$\mu_{k_0}^k = (\psi_{k_0}, \mu\psi_k)_X \neq 0 \text{ for all } k = 1, 2, \dots, \tag{2.49}$$

where ψ_k is the k-th eigenstate of $\mathcal{H}_0$, and that

$$\{S(t)\Psi_0,\ t \geq 0\} \text{ compact in } X. \tag{2.50}$$

Assumption (2.50) holds, for example, if $dom(\mathcal{H}_0)$ is compact in H and $\psi_0 \in V \times V$. In case Ω is unbounded we may assume that $W = V \times L^p(\Omega), p > 2$, is compactly embedded in $H = L^2(\Omega)$. Then, if $\Psi_0 \in W \times W$ and $S(t)$ leaves $W \times W$ invariant [29], we have (2.50).

Since $V(t) \geq 0$, it follows from (2.33) that either $V(t) \to \infty$ or $\int_0^\infty |u(t)|\, dt < \infty$. We also assume that

$$\int_0^\infty |\epsilon(t)|\, dt < \infty. \tag{2.51}$$

This assumption holds if either we use the regularized feedback law (2.32) for arbitrary $\delta > 0$ or $\beta = 0$. Thus,

$$\lim_{t\to\infty} \int_0^t S(t-s)\epsilon(s)B\Psi(s)\, ds \text{ exists.}$$

By Dominated Convergence Theorem [18]. Then it follows that $\{\int_0^t S(t-s)\epsilon(s)B\psi(s) : t \geq 0\}$ is compact in $H \times H$. Together with (2.50) we conclude that $\{\Psi(t) : t \geq 0\}$

is compact. We shall proceed with the asymptotic analysis utilizing assumptions (2.49)–(2.50) and summarize the results in a theorem at the end. Our analysis is based on a type of invariance principle.

Since $\{\Psi(t) : t \geq 0\}$ and $\{\mathcal{O}(t) : t \geq 0\}$ are compact in X there exists a sequence $\{t_n\} \to \infty$ and elements $\Psi_\infty \in X$, $\mathcal{O}_\infty \in X$ such that

$$\lim_{n\to\infty} \Psi(t_n) = \Psi_\infty \text{ and } \lim_{n\to\infty} \mathcal{O}(t_n) = \mathcal{O}_\infty, \tag{2.52}$$

in particular, $\Psi_\infty, \mathcal{O}_\infty$ are in the $\omega-$ limit points of the flow defined by (2.29) and (2.30), respectively. Since $\epsilon \in L^2(0,\infty)$ it follows from (2.28) that $\Psi(t_n + \tau) \to S(\tau)\Psi_\infty$ and analogously $\mathcal{O}(t_n + \tau) \to S(\tau)\mathcal{O}_\infty$ uniformly with respect to $\tau \in (0,\infty)$. Here $S(\tau)\Psi_\infty$ and $S(\tau)\mathcal{O}_\infty$ are the mild solutions to

$$\frac{d}{dt}\Psi_\infty(t) = A_0\Psi_\infty(t), \quad \Psi_\infty(0) = \Psi_\infty,$$

$$\frac{d}{dt}\mathcal{O}_\infty(t) = A_0\mathcal{O}_\infty(t), \quad \mathcal{O}_\infty(0) = \mathcal{O}_\infty.$$

Moreover

$$\Psi_\infty(\tau) = \sum_{k=1}^{\infty} A_k e^{-i(\lambda_k\tau - \theta_k)}\psi_k,$$

$$\mathcal{O}_\infty(\tau) = e^{-i(\lambda_{k_0}\tau - \tilde{\theta}_{k_o})}\psi_{k_0},$$

with $0 \leq \theta_k,\ \tilde{\theta}_{k_0} < \pi$ and $\sum |A_k|^2 = 1$. Since

$$u(t_n + \cdot) = \operatorname{Im}(\mathcal{O}(t_n + \cdot), \mu\Psi(t_n + \cdot) \to 0 \text{ in } L^2(0,\infty),\ \text{as } t_n \to \infty,$$

we have

$$u(\tau) = \operatorname{Im}(\mathcal{O}_\infty(\tau), \mu\Psi_\infty(\tau)) = 0,\ \text{for } \tau \geq 0. \tag{2.53}$$

It follows now that

$$u(\tau) = \operatorname{Im}(\sum_{k=1}^{\infty} A_k e^{i((\lambda_k - \lambda_{k_0})\tau - \theta_k + \tilde{\theta}_{k_0}))}\mu_{k_0}^k)$$

$$= \sum_{k=1}^{\infty} \mu_{k_0}^k A_k \Big(\cos(\theta_k - \tilde{\theta}_{k_0})\sin((\lambda_k - \lambda_{k_0})\tau) - \sin(\theta_k - \tilde{\theta}_{k_0})\cos((\lambda_k - \lambda_{k_0})\tau)\Big) = 0. \tag{2.54}$$

Suppose the family

$$\{\cos((\lambda_k - \lambda_{k_0})\tau), \sin((\lambda_k - \lambda_{k_0})\tau)\} \text{ is } \omega- \text{ independent in } L^2(0,T), \tag{2.55}$$

i.e., a family $\{\varphi_k\}_{k=-\infty}^{\infty}$ is called ω-independent if $\sum_{k=-\infty}^{\infty} c_k\varphi_k = 0$ implies that $c_k = 0$ for all k. Then, $\mu_{k_0}^k A_k = 0$ for $k \neq k_0$ and $\mu_{k_0}^{k_0} A_{k_0} - \sin(\theta_k - \tilde{\theta}_{k_0}) = 0$, Thus, by (2.49) $A_k = 0$ for $k \neq k_0$. Moreover, since $|\Psi_\infty| = 1$, we have $\theta_{k_0} = \tilde{\theta}_{k_0}$ and $A_{k_0} = 1$. Here the case $A_{k_0} = -1$ can be excluded since it implies that

$$V(\Psi_\infty(\tau), \mathcal{O}_\infty(\tau)) = 1 + \mathrm{Re}\,(e^{-i(\lambda_{k_0}\tau - \theta_{k_0})}\psi_{k_0}, e^{-i(\lambda_{k_0}\tau-\theta_{k_0})}\psi_{k_0})_X = 2,$$

and

$$V_1(\Psi_0, \mathcal{O}(0)) = 1 - \mathrm{Re}\big(e^{i\tilde{\theta}_{k_0}}\psi_{k_0}, \Psi_0\big)_X = 1 - Re\big(e^{i\tilde{\theta}_{k_0}}(\psi_{k_0}, \Psi_0)_X\big) < 2,$$

since $\tilde{\theta}_{k_0} \in [0, \pi)$. Hence, $A_{k_0} = -1$ is impossible since $\frac{d}{dt}V(\Psi(t), \mathcal{O}(t)) \leq 0$.

Since the ω-limit pair $(\Psi_\infty, \mathcal{O}_\infty)$ was arbitrary, it follows from (2.18) that $\lim_{t\to\infty} V(\Psi(t), \mathcal{O}(t)) = 0$, i.e. $\Psi(t)$ asymptotically approaches the orbit $\mathcal{O}(t)$. We summarize the above discussion as;

Theorem 2.6.1 *Assume the following conditions holds:*

1. $\mu_{k_0}^k = (\psi_{k_0}, \mu\psi_k)_X \neq 0$ *for all* $k = 1, 2, \ldots,$
2. $\{S(t)\Psi_0,\ t \geq 0\}$ *is compact in* X,
3. $\{\cos((\lambda_k - \lambda_{k_0})\tau), \sin((\lambda_k - \lambda_{k_0})\tau)\}$ *is* $\omega-$ *independent in* $L^2(0,T)$.

then $\Psi(t)$ *asymptotically approaches to the orbit* $\mathcal{O}(t)$,

$$\lim_{t\to\infty} V(\Psi(t), \mathcal{O}(t)) = 0$$

by the nonlinear feedback law (2.23).

In practice, the condition (2.55) is not easy to verify. Hence the following lemma gives an equivalent form for the condition (2.55). It will be called as the gap condition.

Lemma 2.6.1 *If there exits a constant* $\delta > 0$ *such that* $|\lambda_k + \lambda_\ell - 2\lambda_{k_0}| \geq \delta$ *for all* $k, \ell \geq 1$ *with* $\ell \neq k_0$, *and* $|\lambda_k - \lambda_\ell| \geq \delta$ *for all* $k \neq \ell$, *then* $\{e^{i(\lambda_k - \lambda_{k_0})\tau}\} \cup \{e^{-i(\lambda_k-\lambda_{k_0})\tau}\}_{k\neq k_0}$ *is* $\omega-$ *independent for sufficiently large* $T > 0$.

Proof: Let $\{\mu_\ell\}_{\ell\in I}$ be a real number sequence defined by

$$\mu_k = \lambda_k - \lambda_{k_0}, \quad k \geq 1, \quad \mu_{-k} = -(\lambda_k - \lambda_{k_0}) \;\; k \neq k_0.$$

It follows from the assumption that

$$|\mu_m - \mu_\ell| \geq \delta, \quad m \neq \ell$$

From the Ingham's theorem [28], if $T > \frac{2\pi}{\delta}$, there exits a constant c, depending on T and $\delta > 0$ such that

$$c \sum_{m\in I} |a_m|^2 \leq \int_0^T |f(\tau)|^2 \, d\tau$$

for

$$f(\tau) = \sum_{m\in I} a_m e^{i\mu_m \tau}.$$

This implies if $f(\tau) = 0$, then all the coefficient $a_m = 0$ for $m \in I$.

Remark 2.6.1 For the harmonic oscillator case we have

$$\mathcal{H}_0\psi = -\frac{d^2}{dx^2}\psi + x^2\psi, \quad x \in \mathbb{R} = \Omega. \tag{2.56}$$

Then the eigen-pairs $\{(\lambda_k, \psi_k)\}_{k=1}^{\infty}$ are given by

$$\lambda_k = 2k - 1, \quad \psi_k(x) = \hat{c}\, H_{k-1}(x) e^{-\frac{x^2}{2}}$$

where H_k is the Hermite polynomial of degree k and $\hat{c}$ is a normalizing factor. In this case we have

$$\lambda_{k_0-\ell} - \lambda_{k_0} = -(\lambda_{k_0+\ell} - \lambda_{k_0}), \quad 1 \leq \ell \leq k_0 - 1,$$

and the gap condition $|\lambda_k + \lambda_\ell - 2\lambda_{k_0}| > \delta$ is not satisfied. Thus, $\displaystyle\int_0^T |u(\tau)|^2 \, d\tau = 0$ implies

$$\mathrm{Im}\,(A_{k_0+\ell} e^{i(\lambda_\ell\tau - \theta_{k_0+\ell} + \tilde{\theta}_{k_0})} \mu_{k_0}^{k_0+\ell} + A_{k_0-\ell} e^{-i(\lambda_\ell\tau - \theta_{k_0-\ell} + \tilde{\theta}_{k_0})} \mu_{k_0}^{k_0-\ell}) = 0$$

for $1 \leq \ell < k_0$. That is, $A_{k_0-\ell}$ and $A_{k_0-\ell}$ are not necessary zero and thus $\Psi_\infty(\tau)$ is distributed over energy levels $1 \leq \ell \leq 2k_0 - 1$.

We now turn to the case when the gap condition $|\lambda_k + \lambda_\ell - 2\lambda_{k_0}| > \delta$ is violated. Then more than one control operator μ is required and we consider the multiple control potentials (2.25). For the Lyapunov functional $V(\Psi, \mathcal{O}) = 1 - \mathrm{Re}\,(\mathcal{O}, \Psi)_X$, we find

$$\frac{d}{dt}V(\Psi(t), \mathcal{O}(t)) = \sum_{j=1}^{m} \epsilon_j Im(\mathcal{O}(t), \mu_j \Psi(t))_X,$$

which suggests feedback laws of the form

$$\epsilon_j(t) = -\frac{1}{\alpha}(u_j(t) + \beta\,\mathrm{sign}(u_j(t))V(t)^\gamma), \quad u_j(t) = \mathrm{Im}\,(\mathcal{O}(t), \mu_j \Psi(t)). \tag{2.57}$$

As shown above, we have

$$V(t) - V(0) = -\frac{1}{\alpha}\int_0^t \sum_{j=1}^{m}(|u_j(s)|^2 + \beta\,|u_j(s)|V(s)^\gamma)\,ds.$$

In the following discussion we assume (2.50) i.e. that $\{S(t)\Psi_0 : t \geq 0\}$ is compact. Then using the same arguments as above for all $\omega-$ limits $\{\Psi_\infty(\tau) : \tau \geq 0\}$ we have

$$u_j(\tau) = \mathrm{Im}\big(\mathcal{O}_\infty(\tau), \mu_j \Psi_\infty(\tau)\big) = 0, \text{ for } \tau \geq 0, j = 1, \ldots, m.$$

Thus,

$$\mathrm{Im}\Big(\sum_{k=1}^{\infty} A_k e^{i((\lambda_k - \lambda_{k_0})\tau - \theta_k + \tilde{\theta}_{k_0})}(\mu_j)_{k_0}^k\Big) = 0, \text{ for } j = 1, \ldots, m,$$

where

$$(\mu_j)_{k_0}^k = (\psi_{k_0}, \mu_j \psi_k)_X.$$

We henceforth consider the case $m = 2$, that is, two control potentials. Suppose that $\lambda_{\bar{k}} + \lambda_{\bar{\ell}} - 2\lambda_{k_0} = 0$ for a single pair $(\bar{k}, \bar{\ell})$, $\bar{\ell} \neq k_0$, and otherwise (2.55) holds. Then $\lambda_{\bar{k}} - \lambda_{k_0} = -(\lambda_{\bar{\ell}} - \lambda_{k_0})$ and we have

$$\mathrm{Im}\,\big(A_{\bar{k}} e^{i((\lambda_{\bar{k}} - \lambda_{k_0})\tau - \theta_{\bar{k}} + \tilde{\theta}_{k_0})}(\mu_j)_{k_0}^{\bar{k}} + A_{\bar{\ell}} e^{i(-(\lambda_{\bar{k}} - \lambda_{k_0})\tau - \theta_{\bar{\ell}} + \tilde{\theta}_{k_0})}(\mu_j)_{k_0}^{\bar{\ell}}\big) = 0, \tag{2.58}$$

for $j = 1,\ 2$. If

$$\mathrm{rank}\begin{pmatrix} (\mu_1)_{k_0}^{\bar{k}} & (\mu_1)_{k_0}^{\bar{\ell}} \\ \\ (\mu_2)_{k_0}^{\bar{k}} & (\mu_2)_{k_0}^{\bar{\ell}} \end{pmatrix} = 2, \tag{2.59}$$

then from (2.58), it follows that $A_{\bar{k}} = A_{\bar{\ell}} = 0$. If moreover

$$\text{for each } k \text{ there exists } j \in \{1, 2\} \text{ such that } (\mu_j)_{k_0}^k \neq 0, \tag{2.60}$$

then $A_k = 0$ for all $k \neq k_0$, $A_{k_0} = 1$ and $\theta_{k_0} = \tilde{\theta}_{k_0}$. Hence we have $\lim_{t\to\infty} V(\Psi(t), \mathcal{O}(t)) = 0$.

In general let

$$\lambda_{k_i} + \lambda_{\ell_i} - 2\lambda_{k_0} = 0$$

for multiple pairs (k_i, ℓ_i) with $\ell_i \neq k_0$. If

$$\operatorname{rank} \begin{pmatrix} (\mu_1)^{k_i}_{k_0} & (\mu_1)^{\ell_i}_{k_0} \\ \\ (\mu_2)^{k_i}_{k_0} & (\mu_2)^{\ell_i}_{k_0} \end{pmatrix} = 2 \tag{2.61}$$

for each i, then $A_{k_i} = A_{\ell_i} = 0$, and in particular $A_k = 0$ for all k. If in addition (2.60) holds then, again $\lim_{t\to\infty} V(\Psi(t), \mathcal{O}(t)) = 0$.

To summarize, if the gap condition is violated, more than one control potential is required to have asymptotic tracking properties by the feedback law (2.22), provided that the rank condition (2.61) is satisfied.

2.7 Numerical Results

In this section we demonstrate the feasibility of our proposed feedback laws using a test example. We set $H = L^2(0,1)$ and

$$\mathcal{H}_0\psi = \sum_{k=1}^{\infty} \lambda_k (\psi, \psi_k)_H \, \psi_k,$$

where

$$\psi_k(x) = \sqrt{2}\sin(k\pi x) \quad \text{and} \quad \lambda_k = k\pi.$$

Note that this Hamiltonian $\mathcal{H}_0$ is typologically same as the harmonic oscillator (2.56). In order to have asymptotic tracking properties, we test with two control potentials. The control Hamiltonians are given by

$$(\mu_i\Psi)(x) = b_i(x)\Psi(x), \quad x \in (0,1),$$

with $i = 1, 2$. For computations we truncated the expansion of $\mathcal{H}_0$ at $N = 99$, so that

$$S_N(h)\Psi_0 = \sum_{k=1}^{N} e^{-i\lambda_k h} (\Psi_0, \psi_k) \, \psi_k.$$

To integrate the control Hamiltonian term the collocation method was used in the form

$$(B_i^N \psi)(x_n^N) = b_i(x_n^N)\psi(x_n^N), \quad i = 1,\ 2,$$

where $x_n^N = \frac{n}{N},\ 1 \le n \le N-1$. Thus, we implemented the feedback law based on the Strang splitting method in the form

$$\Psi^{k+1} = S_N(\tfrac{h}{2})\mathcal{F}_N(I - \epsilon_1^k \tfrac{h}{2} B_1^N - \epsilon_2^k \tfrac{h}{2} B_2^N)^{-1}(I + \epsilon_1^k \tfrac{h}{2} B_1^N + \epsilon_2^k \tfrac{h}{2} B_2^N) S_N(\tfrac{h}{2})$$

$$\epsilon_i^k = F_i(\Psi^{k+1/2}, \mathcal{O}^{k+1/2}), \quad i = 1,\ 2,$$

where $\mathcal{F}_N$ and $\mathcal{F}_N^{-1}$ are the discrete Fourier sine transform and its inverse transform, respectively and B_i^N is the diagonal matrix with diagonal

$$(b_i(x_1^N), \cdots, b_i(x_{N-1}^N) \quad \text{for each } i = 1,\ 2.$$

This is an implicit method and its well-posedness is discussed in Section 2.5 for given $\beta > 0$ and $\gamma \in [0, 1]$. The numerical tests that we report on are computed with step size $h = 0.01$, $\alpha = 1/500$ and

$$b_1(x) = (x - .5) + 1.75(x - .5)^2, \quad b_2(x) = 2.5(x - .5)^3 - 2.5(x - .5)^4.$$

These control potentials satisfy the rank condition in Section 2.6 and are selected by minimizing the tracking time by trial and error tests. Figure 2.1 and Figure 2.2 shows the orbit tracking performance $V = \frac{1}{2}|\Psi(t) - \mathcal{O}(t)|_X^2$ comparison between different β and different power γ of V. As β increases, the performance V is significantly improved and it can be seen that 10 % performance level is achieved in much shorter horizon. By decreasing the power of V, the performance V improves also and is more rapidly decreased at the beginning of the time horizon.

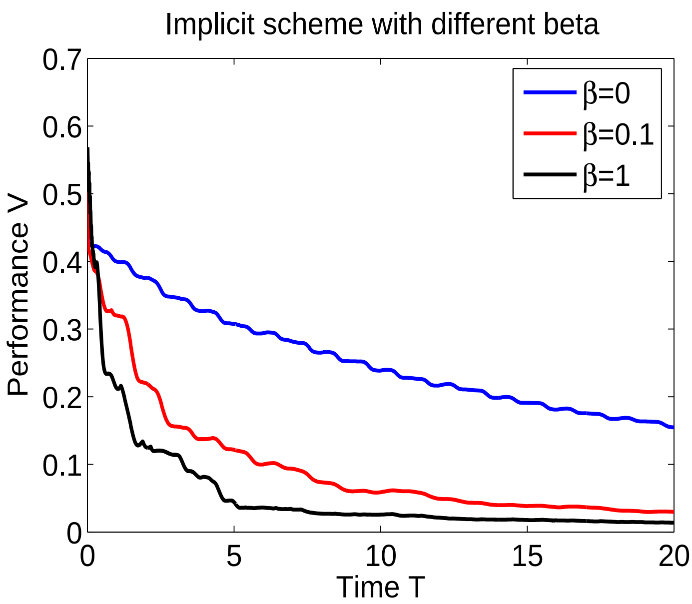

Figure 2.1: Tracking performance comparison for different β

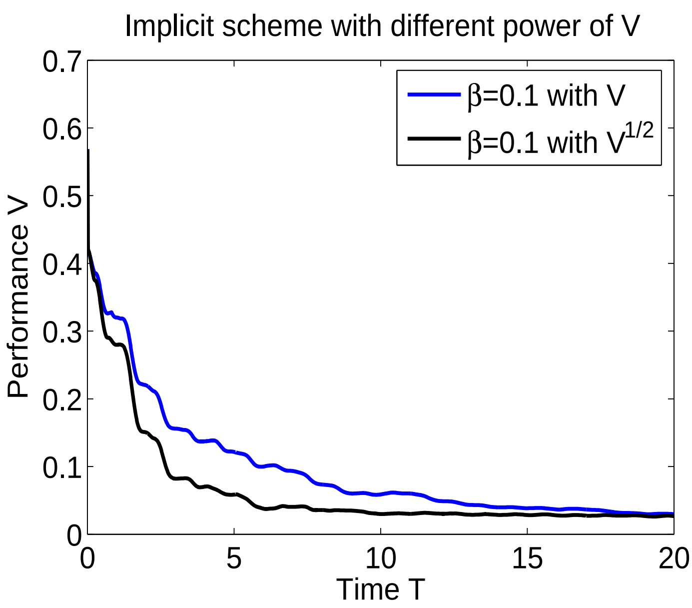

Figure 2.2: Tracking performance comparison for different γ

Chapter 3

Receding Horizon Control Synthesis

In this section, the receding horizon control synthesis is applied to improve the performance of the feedback law in Chapter 2. We formulate the optimality system of optimal control problem on each receding horizon and apply monotone scheme to solve the optimality system iteratively.

3.1 Introduction

Receding horizon control (RHC), also referred to as model predictive control (MPC) is a time-decomposition technique for the longer horizon, which has been widely used in industry. It introduces a new concept of the receding horizon, since the horizon recedes as time proceeds.

Receding horizon control is based on repeatedly solving a series of optimal control problems starting from the current state. Instead of solving on a long horizon directly, RHC divide long horizon into smaller horizons and solve optimal control problem on each smaller horizon sequentially. The concept of RHC can be described as follows. At the current time, optimal controls are obtained on a fixed finite horizon from the current time s, say $[s, s+T]$ by solving the following optimization problem.

$$\min \quad \int_s^{s+T} h(x(t)) + \frac{|u(t)|^2}{2}\, dt + g(x(s+T))$$

subject to the dynamics

$$\frac{d}{dt}x(t) = f(x(t), u(t))$$

where $x(t) \in X$ is the state variable, and $h : X \to \mathbb{R}$, $g : X \to \mathbb{R}$. Among the optimal controls on the fixed finite horizon $[s, s+T]$, only the first one is implemented as the current control law on horizon $[s, s+\Delta]$. Then the same procedure is repeated at time $s+\Delta$ over the next horizon say $[s+\Delta, s+T+\Delta]$ until reaching the final time. In fact, the RHC uses the information of the future horizon T to make a better decision at current time s than simply using current information alone.

There are several advantages of RHC. For example, it has closed-loop structure, guaranteed stability, good tracking performance, and has an easy extension to nonlinear systems. For a complete description of RHC, we refer to [36].

3.2 Receding Horizon Control Method

For the orbit tracking problem of the Schrödinger equation, the objective is to control the state function $\Psi(x,t)$ to the uncontrolled dynamics $\mathcal{O}(x,t)$. For a fixed horizon say $[0, T_f]$, the performance of control strategy can be evaluated by the criterion, how close $\Psi(x,t)$ is to $\mathcal{O}(x,t)$. This quantity can be measured by the Lyapunov functional

$$V(t) = \frac{1}{2}\left|\Psi(t) - \mathcal{O}(t)\right|_X^2.$$

At terminal time T_f, we want the quantity $V(T_f)$ as small as possible. To achieve this, we apply the receding horizon synthesis.

As discussed in section 3.1, receding horizon synthesis is based on solving a series of optimal control problem on the receding horizon. Consider the sequence of the finite horizon optimization problem on $[T_i, T_i + T]$,

$$\min \quad J(\epsilon) = \int_{T_i}^{T_i+T} \frac{1}{2}(|\Psi(t) - \mathcal{O}(t)|^2 + \alpha\,|\epsilon(t)|^2)\,dt + \frac{1}{2}|\Psi(T_i+T) - \mathcal{O}(T_i+T)|^2 \qquad (3.1)$$

subject to (2.14), that is,

$$\frac{d}{dt}\Psi(t) = A\Psi(t) + \epsilon(t)B\Psi(t), \quad \Psi(T_i) = \text{given} \qquad (3.2)$$

In the cost functional (3.1), the orbit tracking is performed not only at the terminal time $T_i + T$, but also at every intermediate time. By including the term $\frac{1}{2}(|\Psi(t) - \mathcal{O}(t)|^2$ inside the integral, we have better tracking performance than without including it.

Here we present two types of receding horizon synthesis.

I (Instantaneous Receding Horizon) Given $\Psi(T_i)$ we compute the optimal control ϵ_i for problem (3.1) on the horizon $[T_i, T_i + k\Delta T],\ k \geq 1$ and then execute the control only on the first step horizon $[T_i, T_i+\Delta T]$, where $\Delta T > 0$ is small and denotes the execution duration. In this case, the receding horizon $T = k\Delta T$ and k is called receding step.

II (Regular Receding Horizon) Given $\Psi(T_i)$ we compute the optimal control ϵ_i on the horizon $[T_i, T_i + T]$ and then execute the control on the whole horizon $[T_i, T_i + T]$, where T is relative large. In this case, once the optimal problem for the previous T horizon is solved, we forward to the next T horizon.

As we can see, the difference between these two receding horizon synthesis lies on how to execute the optimal control computed on the receding horizon $[T_i, T_i + T]$. Type I receding executes the control only on the first step, while Type II receding executes the control on the whole receding horizon. In any case the receding horizon synthesis is a feedback control in the sense that ϵ_i on $[T_i, T_i + T]$ is a function of $\Psi(T_i)$.

To compute the receding horizon synthesis, it is necessary to solve the optimization problem (3.1) on each horizon $[T_i, T_i+T]$. Followed by the Pontryagin Maximum Principle, the necessary optimality condition for (3.1) (3.2) is given by

$$
\begin{aligned}
&\tfrac{d}{dt}\Psi(t) = (A + \epsilon(t)B)\Psi(t), \quad \Psi(T_i) = \text{given};\\
&-\tfrac{d}{dt}\chi(t) = (A + \epsilon(t)B)^*\chi(t) - \mathcal{O}(t), \quad \chi(T_i + T) = \mathcal{O}(T_i + T);\\
&\epsilon(t) = \tfrac{1}{\alpha}(B\Psi(t), \chi(t)).
\end{aligned}
\tag{3.3}
$$

where the function $\chi(t)$ is the costate associated to the state function $\Psi(t)$ and the control $\epsilon(t)$ is computed based on $\chi(t)$ instead of the orbit $\mathcal{O}(t)$. Starting from the feedback solution $\tilde{\epsilon}^0 = F(\Psi(t), \mathcal{O}(t))$ in (2.22), we apply the following iterative method to solve the two-point boundary value problem (3.3). The scheme is as follows:

$$
\begin{aligned}
&\frac{d}{dt}\Psi^{k+1} = (A + \epsilon^{k+1}\, B)\Psi^{k+1}, \quad \Psi^{k+1}(T_i) = \text{given} \\
&\epsilon^{k+1} = (1-\delta)\tilde{\epsilon}^{k} + \frac{\delta}{\alpha}(B\Psi^{k+1}, \chi^{k}) \\
&-\frac{d}{dt}\chi^{k+1} = (A + \tilde{\epsilon}^{k+1}\, B)^{*}\chi^{k+1} + \mathcal{O}(t), \quad \chi^{k+1}(T_i + T) = \mathcal{O}(T_i + T) \\
&\tilde{\epsilon}^{k+1} = (1-\eta)\epsilon^{k+1} + \tfrac{\eta}{\alpha}(B\Psi^{k+1}, \chi^{k+1})
\end{aligned}
\tag{3.4}
$$

where $\delta,\ \eta \in (0,2)$ is the relaxization parameters, and k is the number of iteration. The initialization is given by

$$\tilde{\epsilon}^{0} = F(\Psi(t), \mathcal{O}(t)) \quad \text{and} \quad \chi^{0}(t) = \mathcal{O}(t).$$

The scheme (3.4) can be described as follows: Starting at iteration $k = 1$, we solve an initial value problem for Ψ forward with control given by feedback solution $\epsilon^{1} = \tilde{\epsilon}^{0}$ until reaching terminal time $T_i + T$; then solve the adjoint equation for χ backwards to the initial time T. This process is repeated to solve the state and costate forwards and backwards sequentially.

It has been proved in [29] that

$$J(\epsilon^{k-1}) - J(\epsilon^{k}) = \frac{\alpha}{2}\int_{T_i}^{T_i+T} (\frac{2}{\delta} - 1)\,|\epsilon^{k} - \tilde{\epsilon}^{k-1}|^2 + (\frac{2}{\eta} - 1)\,|\epsilon^{k-1} - \tilde{\epsilon}^{k-1}|^2\, dt.$$

That is, one can improve the tracking performance as the number of iterates increases. Hence (3.4) is called the monotone scheme. Similar description of the monotone scheme can be found in [74] [49].

In summary, to use receding horizon synthesis to improve tracking performance, we apply the monotone scheme (3.4) to solve a sequence of receding horizon control problem (3.1) on $[T_i, T_i + T]$ starting with the feedback solution $\bar{\epsilon}(t)$ to get an optimal pair (ϵ^{*}, Ψ^{*}). Then we apply the control ϵ^{*} on $[T_i, T_i + \Delta T]$ and set $\Psi(T_{i+1}) = \Psi^{*}(T_i + \Delta T)$. For Type I short receding, $T = k\Delta T$, where k is called the receding step. While for Type II long receding, $\Delta T = T$.

3.3 Time Discretization

In this section we discuss the time-discretization of optimization problem (3.1) (3.2) using the splitting method (2.42).

Consider the problem to minimize

$$J_h(\epsilon) = \frac{1}{2}|\Psi_m - \mathcal{O}_m|^2 + \Delta t \sum_{j=0}^{m-1} (\frac{\alpha}{2}|\epsilon_j|^2 + \frac{1}{2}(\hat{\Psi}_{j+1} - \mathcal{O}_{j+1/2}|^2 + |\hat{\Psi}_j - \mathcal{O}_{j+1/2}|^2)), \quad (3.5)$$

subject to (2.42);

$$\hat{\Psi}_j = S(\frac{h}{2})\Psi_j, \quad \frac{\hat{\Psi}_{j+1} - \hat{\Psi}_j}{\Delta t} = \epsilon_j\, B\frac{\hat{\Psi}_{j+1} + \hat{\Psi}_j}{2}, \quad \Psi_{j+1} = S(\frac{h}{2})\hat{\Psi}_{j+1}. \quad (3.6)$$

Define the Lagrangian

$$L(\epsilon, \Psi, \chi) = J_h(\epsilon) + \sum_{j=0}^{m-1} \frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2}(\frac{\hat{\Psi}_{j+1} - \hat{\Psi}_j}{\Delta t} - \epsilon_j B\frac{\hat{\Psi}_{j+1} + \hat{\Psi}_j}{2})\Delta t.$$

set $\frac{\partial L}{\partial \hat{\Psi}_j} = 0$, we get

$$-\mathcal{O}_{j+\frac{1}{2}}\Delta t + \frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2}(-\frac{1}{\Delta t} - \frac{\epsilon_j B^*}{2})\Delta t + \frac{\hat{\chi}_{j-1} + \hat{\chi}_j}{2}(\frac{1}{\Delta t} - \frac{\epsilon_{j-1}B^*}{2})\Delta t = 0$$

$$-\frac{\hat{\chi}_j - \hat{\chi}_{j-1}}{\Delta t} - \epsilon_{j-1}B^*\frac{\hat{\chi}_{j-1} + \hat{\chi}_j}{2} - \mathcal{O}_{j+\frac{1}{2}} + \frac{\hat{\chi}_{j-1} - \hat{\chi}_j}{\Delta t} - \epsilon_j B^*\frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2} - \mathcal{O}_{j+\frac{1}{2}} = 0$$

hence

$$-\frac{\hat{\chi}_j - \hat{\chi}_{j+1}}{\Delta t} = \epsilon_j B^*\frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2} + \mathcal{O}_{j+1/2}$$

set $\frac{\partial L}{\partial \epsilon_j} = 0$, we get

$$\alpha\Delta t\epsilon_j - (\frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2}, B\frac{\hat{\Psi}_j + \hat{\Psi}_{j+1}}{2})\Delta t = 0$$

$$\epsilon_j = \frac{1}{\alpha}(B\frac{\hat{\Psi}_{j+1} + \hat{\Psi}_j}{2}, \frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2})$$

Thus, we obtain the necessary optimality condition for the time-discretization system (3.5) (3.6),

$$\hat{\Psi}_j = S(\frac{h}{2})\Psi_j, \quad \frac{\hat{\Psi}_{j+1} - \hat{\Psi}_j}{\Delta t} = \epsilon_j\, B\frac{\hat{\Psi}_{j+1} + \hat{\Psi}_j}{2}, \quad \Psi_{j+1} = S(\frac{h}{2})\hat{\Psi}_{j+1}.$$

$$\hat{\chi}_{j+1} = S(\frac{h}{2})^*\chi_{j+1}, \quad -\frac{\hat{\chi}_j - \hat{\chi}_{j+1}}{\Delta t} = \epsilon_j B^*\frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2} + \mathcal{O}_{j+1/2}, \quad \chi_j = S(\frac{h}{2})^*\hat{\chi}_j$$

$$\epsilon_j = \frac{1}{\alpha}(B\frac{\hat{\Psi}_{j+1} + \hat{\Psi}_j}{2}, \frac{\hat{\chi}_j + \hat{\chi}_{j+1}}{2})$$

The corresponding monotone scheme is given by

$$\hat{\Psi}_j^{k+1} = S(\frac{h}{2})\Psi_j^{k+1}, \quad \frac{\hat{\Psi}_{j+1}^{k+1} - \hat{\Psi}_j^{k+1}}{\Delta t} = \epsilon_j^{k+1} B\frac{\hat{\Psi}_{j+1}^{k+1} + \hat{\Psi}_j^{k+1}}{2}, \quad \Psi_{j+1}^{k+1} = S(\frac{h}{2})\hat{\Psi}_{j+1}^{k+1},$$

$$\epsilon_j^{k+1} = (1-\delta)\tilde{\epsilon}_j^k + \frac{\delta}{\alpha}(B\frac{\hat{\Psi}_j^{k+1} + \hat{\Psi}_{j+1}^{k+1}}{2}, \frac{\hat{\chi}_j^k + \hat{\chi}_{j+1}^k}{2}),$$

$$\hat{\chi}_{j+1}^{k+1} = S(\frac{h}{2})^*\chi_{j+1}^{k+1}, \quad -\frac{\hat{\chi}_j^{k+1} - \hat{\chi}_{j+1}^{k+1}}{\Delta t} = \tilde{\epsilon}_j^{k+1} B^*\frac{\hat{\chi}_j^{k+1} + \hat{\chi}_{j+1}^{k+1}}{2} + \mathcal{O}_{j+1/2}, \quad \chi_j^{k+1} = S(\frac{h}{2})^*\hat{\chi}_j^{k+1},$$

$$\tilde{\epsilon}_j^{k+1} = (1-\eta)\epsilon_j^{k+1} + \frac{\eta}{\alpha}(B\frac{\hat{\Psi}_j^{k+1} + \hat{\Psi}_{j+1}^{k+1}}{2}, B\frac{\hat{\chi}_{j+1}^{k+1} + \hat{\chi}_j^{k+1}}{2}),$$

for $j = 0 \ldots m-1$, where $\Psi_0^{k+1} = \Psi_0$ and $\chi_m^{k+1} = \mathcal{O}_m$.

The following theorem states that the above scheme for the time-discretization system is also a monotone scheme.

Theorem 3.3.1

$$J_h(\epsilon^{k-1}) - J_h(\epsilon^k) = \frac{\alpha\Delta t}{2}\sum_{j=1}^{m}(\frac{2}{\delta} - 1)\,|\epsilon_j^k - \tilde{\epsilon}_j^{k-1}|^2 + (\frac{2}{\eta} - 1)\,|\epsilon_j^{k-1} - \tilde{\epsilon}_j^{k-1}|^2.$$

Proof: Since $|\Psi_j^k| = 1$, $|\mathcal{O}_j| = 1$, we have

$$\begin{aligned} J(\epsilon^{k+1}) - J(\epsilon^k) = &-(\Psi_m^{k+1} - \Psi_m^k, \mathcal{O}_m) - \Delta t \textstyle\sum_{j=0}^{m-1}(\frac{\hat{\Psi}_{j+1}^{k+1}+\hat{\Psi}_j^{k+1}}{2} - \frac{\hat{\Psi}_{j+1}^{k}+\hat{\Psi}_j^{k}}{2}, \mathcal{O}_{j+\frac{1}{2}}) \\ &+\frac{\alpha\Delta t}{2}\sum_{j=0}^{m-1}[|\epsilon_j^{k+1}|^2 - |\epsilon_j^k|^2] \end{aligned}$$

Note that $\Psi_0^k = \Psi_0^{k+1} = \Psi_0$ and we use the following equality:

$$\begin{aligned} &\textstyle\sum_{j=0}^{m-1}(\frac{\widehat{\Psi}_{j+1}-\widehat{\Psi}_j}{\Delta t}, \frac{\widehat{\chi}_{j+1}+\widehat{\chi}_j}{2}) + (\frac{\widehat{\Psi}_{j+1}+\widehat{\Psi}_j}{2}, \frac{\widehat{\chi}_{j+1}-\widehat{\chi}_j}{\Delta t}) \\ &= \sum_{j=0}^{m-1}(\frac{\widehat{\Psi}_{j+1}}{\Delta t}, \widehat{\chi}_{j+1}) - (\frac{\widehat{\Psi}_j}{\Delta t}, \widehat{\chi}_j) \\ &= \frac{1}{\Delta t}((\widehat{\Psi}_m, \widehat{\chi}_m) - (\widehat{\Psi}_0, \widehat{\chi}_0)) = \frac{1}{\Delta t}((\Psi_m, \chi_m) - (\Psi_0, \chi_0)). \end{aligned}$$

Thus, we have

$$
\begin{aligned}
&-(\Psi_m^{k+1}-\Psi_m^k,\mathcal{O}_m)-\Delta t\textstyle\sum_{j=0}^{m-1}(\frac{\hat{\Psi}_{j+1}^{k+1}+\hat{\Psi}_j^{k+1}}{2}-\frac{\hat{\Psi}_{j+1}^{k}+\hat{\Psi}_j^{k}}{2},\mathcal{O}_{j+\frac{1}{2}})\\
&=\Delta t\sum_{j=0}^{m-1}\{B[\epsilon_j^{k+1}\frac{\widehat{\Psi}_j^{k+1}+\widehat{\Psi}_{j+1}^{k+1}}{2}-\epsilon_j^k\frac{\widehat{\Psi}_j^{k}+\widehat{\Psi}_{j+1}^{k}}{2}],\frac{\widehat{\chi}_j^k+\widehat{\chi}_{j+1}^k}{2})\\
&\quad+(\frac{\widehat{\Psi}_j^{k+1}+\widehat{\Psi}_{j+1}^{k+1}}{2}-\frac{\widehat{\Psi}_j^{k}+\widehat{\Psi}_{j+1}^{k}}{2},B\widetilde{\epsilon}_j^k\frac{\widehat{\chi}_j^k+\widehat{\chi}_{j+1}^k}{2})\}\\
&=-\alpha\Delta t\sum_{j=0}^{m-1}\frac{1}{\delta}(\epsilon_j^{k+1}-\widetilde{\epsilon}_j^k,\epsilon_j^{k+1}-(1-\delta)\widetilde{\epsilon}_j^k)+\frac{1}{\eta}(\epsilon_j^k-\widetilde{\epsilon}_j^k,\widetilde{\epsilon}_j^k-(1-\eta)\epsilon_j^k)
\end{aligned}
$$

and hence we have

$$
\begin{aligned}
J(\epsilon^{k+1})-J(\epsilon^k)&=-\alpha\Delta t\sum_{j=0}^{m-1}\frac{1}{\delta}(\epsilon_j^{k+1}-\widetilde{\epsilon}_j^k,\epsilon_j^{k+1}-(1-\delta)\widetilde{\epsilon}_j^k)\\
&\quad+\frac{1}{\eta}(\epsilon_j^k-\widetilde{\epsilon}_j^k,\widetilde{\epsilon}_j^k-(1-\eta)\epsilon_j^k)-\frac{1}{2}|\epsilon_j^{k+1}|^2+\frac{1}{2}|\epsilon_j^k|^2\\
&=-\frac{\alpha\Delta t}{2}\sum_{j=0}^{m-1}(\frac{2}{\delta}-1)|\widetilde{\epsilon}_j^k-\epsilon_j^{k+1}|^2+(\frac{2}{\eta}-1)|\epsilon_j^k-\widetilde{\epsilon}_j^k|^2\le 0.
\end{aligned}
$$

Thus we have a numerical method to solve series of the optimal control problems on each receding horizon.

3.4 Numerical Results

In this section we demonstrate the performance of the receding horizon synthesis using the same test example as in section 2.7. We set $H=L^2(0,1)$ and

$$\mathcal{H}_0\psi=\sum_{k=1}^{\infty}\lambda_k(\psi,\psi_k)_H\,\psi_k,$$

where

$$\psi_k(x)=\sqrt{2}\sin(k\pi x)\quad\text{and}\quad\lambda_k=k\pi.$$

The control Hamiltonians are given by

$$(\mu_i\Psi)(x)=b_i(x)\Psi(x),\quad x\in(0,1),$$

with $i=1,2$. For computations we truncated the expansion of $\mathcal{H}_0$ at $N=99$, so that

$$S_N(h)\Psi_0=\sum_{k=1}^{N}e^{-i\lambda_k h}(\Psi_0,\psi_k)\,\psi_k.$$

where h is the time step. To integrate the control Hamiltonian term the collocation method was used in the form

$$(B_i^N \psi)(x_n^N) = b_i(x_n^N)\psi(x_n^N), \quad i = 1,\ 2,$$

where $x_n^N = \frac{n}{N}$, $1 \le n \le N-1$. The numerical tests that we report on are computed with $h = 0.01$, $\alpha = 1/500$ and control potentials

$$b_1(x) = (x - .5) + 1.75(x - .5)^2, \quad b_2(x) = 2.5(x - .5)^3 - 2.5(x - .5)^4.$$

Figure 3.1 shows the numerical results for the instantaneous receding horizon synthesis on time horizon $[0, 20]$. We observe that that the receding horizon synthesis improves the tracking performance of the nonlinear feedback law significantly. Also it is observed that the performance improves with increasing receding step k.

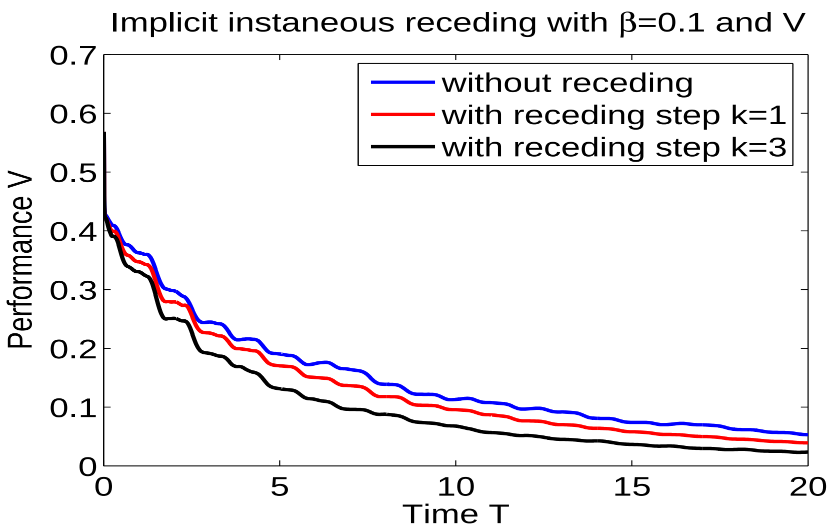

Figure 3.1: Tracking performance of the instantaneous receding horizon control

That is, for a fixed horizon T_f, we can use larger receding step k to achieve better performance in terms of orbit tracking. The mechanism under it is that having a longer receding horizon is using more future information to make better decision at current time. Table 3.1 shows the numerical results.

Figure 3.2 demonstrates the asymptotic orbit tracking for receding horizon synthesis and original feedback law. We see the orbit tracking performance V deceases as time increases for both synthesis, but the receding horizon synthesis performs better. The end per-

Table 3.1: Tracking performance of the receding horizon control with different receding step k.

$T_f = 15$	$\lvert\Psi(T_f) - O(T_f)\rvert^2$
$k = 1$	$5.80 * 10^{-2}$
$k = 2$	$4.62 * 10^{-2}$
$k = 3$	$3.65 * 10^{-2}$
$k = 5$	$2.17 * 10^{-2}$
$k = 10$	$9.09 * 10^{-3}$

formance at $T_f = 200$ for the instantaneous receding horizon control is $V(T_f) = 6.95 * 10^{-4}$ compared with $V(T_f) = 1.49 * 10^{-3}$ for original feedback law. The right side of Figure 3.2 shows the tracked state (real and imaginary parts) after 200 time units compared to the desired orbit. We see that they are very close to each other except some tracked error.

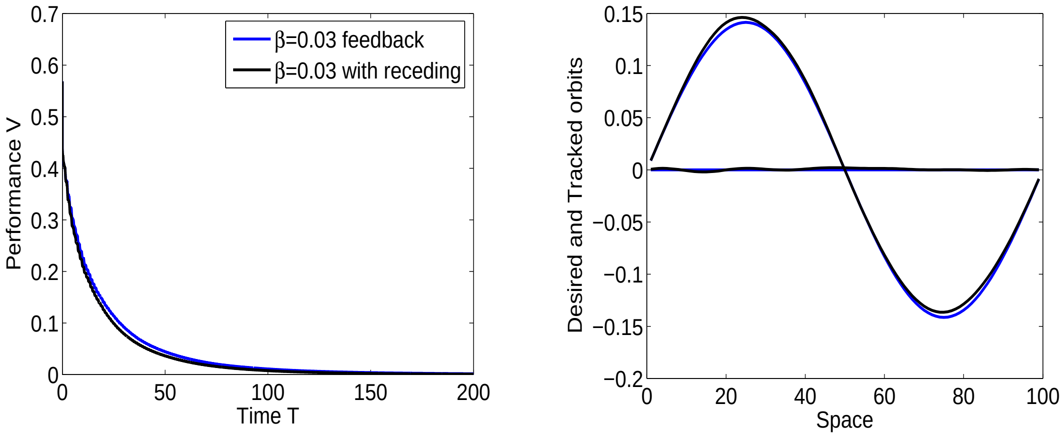

Figure 3.2: Asymptotic orbit tracking

In Section 3.2, we describe applying the monotone scheme (3.4) with relaxation constant $\delta, \eta \in (0, 2)$ to solve the optimality system for the receding horizon control synthesis. As shown in Figure 3.3, we observe that the under-relaxation ($\delta, \eta \in (0, 1)$) performs better than the over-relaxation ($\delta, \eta \in (1, 2)$) .

In Table 3.2 we show numerical results for the tracking performance of regular receding horizon synthesis with different receding horizon T and different numbers of iteration m for the monotone scheme. It is observed that the performance increases with m as the optimality system is solved more exactly. And a longer receding horizon $T = 1$ performs

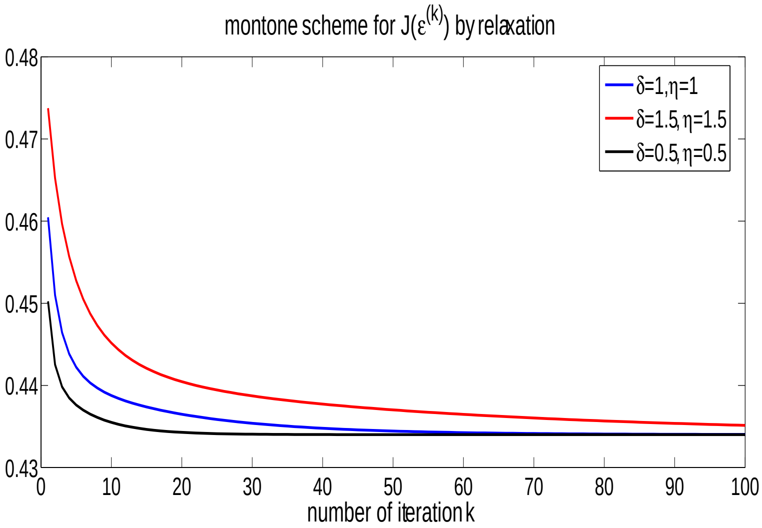

Figure 3.3: $J(\epsilon^{(k)})$ of monotone scheme with different relaxations (δ, η)

Table 3.2: Tracking performance of the regular receding horizon synthesis

$T_f = 200,\ \beta = 0.1$	$\lvert\Psi(T_f) - O(T_f)\rvert^2$
$T = 1,\ m = 1$	$1.60 * 10^{-4}$
$T = 1,\ m = 2$	$8.66 * 10^{-5}$
$T = 0.5,\ m = 1$	$3.14 * 10^{-4}$
without receding	$6.05 * 10^{-4}$

much better than a shorter horizon $T = 0.5$ as should be.

In fact, the regular receding horizon synthesis performs better than the instantaneous receding horizon synthesis but has more computational cost.

Chapter 4

Application to Control of a Tumor Growth Model

In this Chapter, we study the control problem of a tumor growth model, aiming at the reduction of the tumor cells population. By incorporating the switching mechanism, we design an effective feedback law to suppress the tumor growth.

4.1 Introduction

From the twenties century, cancer is one of the main causes of mortality in the world. Developing an effective therapy for the patients is the long term goal. A lot of cancer research has been conducted to find cures and improve existing treatment in the past decades. Thus having a trustful mathematical modeling of tumor growth draws great interest in the mathematical community.

Let us first review the dynamics of tumor growth. Up to now, there is still a lot of controversy over how exactly cancer is initiated, but it is generally accepted that it requires several gene mutations to turn a normal cell into a cancer cell, see [46]. One of the outcomes of this series of mutations is an increase in the proliferation rate and a decrease in the death rate of the cells, giving rise to a clump of tumor cells growing faster than the host cells, which eventually leads to the death of patients. It has been observed in experiment that the tumor cells grow until they reach a critical size when the growth stops. This critical size is determined by a balance between cell proliferation and cell death inside the spheroid. Another main experimental observations have been that when tumor cells are in a high nutrient environment they proliferate, in low nutrient levels the tumor cells trigger cell death, and in intermediate nutrient levels the tumor cells stay quiescent. The different nutrient levels inside the tumor spheroid are determined by the movement and consumption of nutrients within the tumor.

Because there are three distinct stages (avascular, vascular, and metastatic) to cancer development, a lot of research are often concentrated on answering specific questions on each of these stages. In the thesis, we utilize the results about describing the current state of mathematical modeling of avascular tumor growth, i.e., tumors without blood vessels. Although complex in its own right, avascular tumor growth is easier to replicate experimentally, much simpler to model mathematically and yet contains many of the phenomena that researchers and mathematicians will need to address when modeling vascular tumors growth. Hence modeling avascular tumor growth is the first step toward building models for fully vascularized tumors and thus more thoroughly understanding cancer. Our description of the avascular tumor growth model will follow the review paper by T. Roose, S. J. Chapman and P. K. Maini in [60].

The mathematical modeling of tumor growth is to describe the diffusion process of the nutrient within the tumor spheroid. To control the growth of the tumor, it is necessary to maintain a balanced nutrient environment. The process of nutrient consumption and diffusion inside tumors has been modeled since the mid-1960s. Most models fall into two categories: (1) continuum mathematical models, (2) discrete cell population models. In this thesis, our model are based on the continuum mathematical models which consist of partial differential equations, typically reaction-diffusion-convection equations. One of the best parameterized of these models is due to Casciari, Sotirchos, and Sutherland in [13]. Their model considers a spherical tumor and the interaction of tumor cells with oxygen, glucose, lactate, carbon dioxide, and bicarbonate, chloride, and hydrogen ions.

The equations describing the distribution of molecular species inside the tumor spheroid are classical transport/ mass conservation equations. The conservation equations for the different chemical species are

$$\frac{\partial c_i}{\partial t} + \nabla \cdot N_i = P_i \tag{4.1}$$

where $c_i = c_i(t, x)$ are the concentrations of the chemical species, for instance, oxygen, glucose, carbon dioxide, lactate, bicarbonate and hydrogen ion. The location $x \in \Omega \subset \mathbb{R}^3$. N_i is the flux of each of the chemical species inside the tumor spheroid. For simplicity, we assume the flux of all chemical species follows the Fick's law,

$$N_i = -D_i \nabla c_i \tag{4.2}$$

where $D_i > 0$ are constant diffusion coefficients. And P_i is the net rate of consumption or production of the chemical species both by the tumor cells and due to chemical reactions with other species. Hence the dynamics of chemical diffusion can be modeled as

$$\frac{\partial c_i}{\partial t} - D_i \nabla^2 N_i = P_i \tag{4.3}$$

Proliferation gives rise to cell movement. We use $v = v(x, t)$ to denote the velocity of cell movement, which satisfies

$$\nabla \cdot v = \lambda F(c_i) \tag{4.4}$$

where λ is the maximum rate of cell proliferation and $F(c_i)$ is the scaling function for the nutrient/chemical species dependent proliferation.

We consider simple models in which all the cells are tumor cells. Let $u(t, x)$ be an L^2 function on $\mathbb{R}$ to represent the local density of tumor cells at time $t \in [0, \infty]$ and at location $x \in \Omega$, which is a bounded region in $\mathbb{R}^3$. The general mass balance for the tumor can be modeled as

$$\frac{\partial u}{\partial t} + \nabla \cdot (vu) = \nabla \cdot (D \nabla u) + \lambda(u, c) - \mu(u, c) \tag{4.5}$$

here $\lambda(u, c)$ is the chemical dependent cell production, and $\mu(u, c)$ is the chemical dependent cell degradation/death. Due to the interaction and balance of process $\lambda(u, c)$ and $\mu(u, c)$, the tumor cell can be in state of proliferating, quiescent, or necrotic.

To kill the tumor cells or suppress the growth of tumor, anti-angiogenic drug dose will be used. Let $\epsilon(t)$ be the anti-angiogenic drug dose rate, $\chi_\omega(u, c)$ be cell degradation process due to drug dose. The subscript ω denotes a smaller region inside domain Ω where the drug dose is applied. Here we model the local effect of drug dose to the tumor growth. The control problem of the tumor growth is to find a way to control the process of cell degradation/death $\chi_\omega(u, c)$ so as to kill the tumor cells. Our model of the tumor growth control problem is

$$\frac{\partial u}{\partial t} + \nabla \cdot (vu) = \nabla \cdot (D \nabla u) + \lambda(u, c) - \mu(u, c) - \epsilon(t)\chi_\omega(u, c) \tag{4.6}$$

For simplicity, we only consider the linear effect of the cell production/ degradation process $\lambda(u,c)$, $\mu(u,c)$ and $\chi_\omega(u,c)$. It is appropriate to assume they are linear functions of the tumor density $u(t,x)$,

$$\lambda(u,c) = \lambda(c)u, \quad \mu(u,c) = \mu(c)u, \quad \chi_\omega(u,c) = \chi_\omega(c)u$$

The tumor cell can be in the state of quiescence for a balance of chemical consumption and production. That is, the chemical concentration c is in the stationary state, which is time independent. Thus we assume that $\lambda(c)$, $\mu(c)$ and $\chi_\omega(c)$ are time independent. This effect can be rewritten in the form of,

$$\lambda(u,c) - \mu(u,c) = \rho(x)u, \quad \chi_\omega(u,c) = \chi_\omega(x)u$$

where $\rho(x)$ is used to describe the overall cell production/degration for the original uncontrolled system. We further simplify our model to assume that the velocity of cell movement $v = 0$, thus the dynamics of the control process becomes

$$\frac{\partial u(t,x)}{\partial t} = D\nabla^2 u(t,x) + \rho(x)u(t,x) - \epsilon(t)\chi_\omega(x)u(t,x) \tag{4.7}$$

$$u(0,x) = u_0(x) \tag{4.8}$$

for $u(t,x) \in H_0^1([0,\infty) \times \Omega; \mathbb{R})$. The dynamics (4.7) is a bilinear system. The control objective is to find a time dependent control $\epsilon(t) \in L^2(0,\infty)$ which drives $\|u(t)\|_\infty$ close to 0 as t goes to infinity.

From medical experiments, it has been observed that in a biological system, normal cell can live along with the tumor cell. If they are in equilibrium, then it will not harm the health of the patients. If the number of the tumor cell outnumbers the normal cell in certain scale, then the patients will start having bad symptom, then leads to death eventually. Hence the drug usage is not necessary to kill all the tumor cells in the environment, but to depress the growth of the tumor cell to some equilibrium of the system. Once the drug controls the tumor system to certain level, then the nature will take care of it, i.e, the patient will recover himself. Hence instead of controlling the density of tumor cell $u(t)$ to 0, we consider the control problem of driving $u(t)$ to some stable trajectory $\bar{u}(t,x)$ of the dynamics, which has property that $\bar{u}(t,x) \to 0$ as $t \to \infty$.

The stable trajectory $\bar{u}(t,x)$ represents the stable orbit of the uncontrolled dynamics

$$\frac{\partial \bar{u}(t,x)}{\partial t} = D\nabla^2 \bar{u}(t,x) + \rho(x)\bar{u}(t,x) \tag{4.9}$$

corresponds to an eigenstate $\Psi(x)$,

$$D\nabla^2\Psi(x) + \rho(x)\Psi(x) = \lambda\Psi(x) \tag{4.10}$$

for $\lambda < 0$. Then the stable trajectory $\bar{u}(t,x)$ is given by

$$\bar{u}(t,x) = e^{\lambda t}\Psi(x)$$

which decays to 0 as t goes to infinity.

4.2 Feedback Law

In this section, we design a feedback law by Lyapunov techniques. Take a difference between equations (4.7) and (4.9), we have

$$\frac{\partial(u-\bar{u})}{\partial t} = D\nabla^2(u-\bar{u}) + \rho(x)(u-\bar{u}) - \epsilon(t)\chi_\omega(x)u$$

Employing a variational approach based on the Lyapunov functional

$$V(t) = V(u(t),\bar{u}(t)) = \frac{1}{2}\int_\Omega (u(t)-\bar{u}(t))^2 dx \tag{4.11}$$

It can be showed that

$$\begin{aligned}
\frac{dV(t)}{dt} &= \int_\Omega (u-\bar{u})(u-\bar{u})_t dx \\
&= (u-\bar{u})\nabla(u-\bar{u})|_{\partial\Omega} - \int_\Omega D(\nabla(u-\bar{u}))^2 dx \\
&+ \int_\Omega \rho(x)(u-\bar{u})^2 dx - \epsilon(t)\int_\Omega \chi_\omega u(u-\bar{u})dx \\
&= -\int_\Omega D(\nabla(u-\bar{u}))^2 dx + \int_\Omega \rho(x)(u-\bar{u})^2 dx - \epsilon(t)\int_\Omega \chi_\omega u(u-\bar{u})dx
\end{aligned}$$

assuming $u \in H_0^1(\Omega)$ and $\bar{u} \in H_0^1(\Omega)$. In order to control the density of tumor cells $u(t)$ to a stable trajectory $\bar{u}(t)$, we want the derivative of cost functional $V(t)$ as smaller(negative) as possible. Hence we propose the nonlinear feedback law $\epsilon(t)$,

$$\begin{aligned}
&\epsilon(t) = \frac{1}{\alpha}(\eta(t) + \beta\,\mathrm{sign}(\eta(t))V(t)) = F(u(t),\bar{u}(t)), \\
&\eta(t) = \textstyle\int_\Omega \chi_\omega u(u-\bar{u})dx, \quad V(t) = V(u(t),\bar{u}(t)),
\end{aligned} \tag{4.12}$$

for $\alpha > 0$, $\beta \geq 0$. Then

$$\frac{dV(t)}{dt} = -\int_\Omega D(\nabla(u-\bar{u}))^2 dx + \int_\Omega \rho(x)(u-\bar{u})^2 dx - \frac{1}{\alpha}(\eta^2 + \beta|\eta|V) \tag{4.13}$$

Note the fact that, by the proposed feedback law (4.12), the derivative of functional $V(t)$ is not necessarily negative at the beginning, which means $V(t)$ may still increase. But the feedback law can slow down the growth of $u(t,x)$ significantly with the negative term $(\int_\Omega \chi_\omega u(u-\bar{u})dx)^2$. As $u(t,x)$ gets closer and closer to $\bar{u}(t,x)$ as t increase, the term $\int_\Omega \rho(x)(u-\bar{u})^2 dx$ gets smaller and smaller. Then $\frac{dV(t)}{dt}$ can become negative after certain time T. Eventually $u(t,x)$ goes close to $\bar{u}(t,x)$ as $t \to \infty$.

4.3 Numerical Results

The dynamics of the control problem is

$$\frac{\partial u(t,x)}{\partial t} = D\nabla^2 u(t,x) + \rho(x)u(t,x) - \epsilon(t)\chi_\omega(x)u(t,x) \tag{4.14}$$

The Hamiltonian includes two parts

$$H_0 = D\nabla^2, \quad H_1 = \rho(x) - \epsilon(t)\chi_\omega(x)$$

Hence it is natural to use the Strang operator splitting method for the time integration. For the stepsize $\Delta t > 0$,

$$\begin{aligned} \hat{u}_{k+1} &= e^{(\rho-\epsilon_k\chi_\omega)\Delta t}\hat{u}_k, \quad \hat{u}_k = S(\frac{\Delta t}{2})u_k, \\ u_{k+1} &= S(\tfrac{\Delta t}{2})\hat{u}_{k+1}, \end{aligned} \tag{4.15}$$

where

$$\begin{aligned} \epsilon_k &= F(\hat{u}_k, \bar{u}_k) = \tfrac{1}{\alpha}(\eta_k + \beta\,\mathrm{sign}(\eta_k)V_k) \\ \eta_k &= \textstyle\int_\Omega \chi_\omega \hat{u}_k(\hat{u}_k - \bar{u}_k)dx, \quad V_k = V(\hat{u}_k, \bar{u}_k), \end{aligned} \tag{4.16}$$

$S(\frac{\Delta t}{2})$ is the half step time integration for H_0, which we use Fast Fourier Transformation to compute.

The Strang splitting method is of second order as time integration. The solution u_k converges to $u(t)$ uniformly as $\Delta t \to 0$. The proof of the convergence result for (4.15) is similar to the case of control for the Schrödinger equation in Section 2.5.

We demonstrate the feasibility of the control law (4.12) through a 2D test example. The physical domain Ω is $(x, y) \in [0, 1] \times [0, 1]$, the diffusion constant D is set to be 1. In the simulation, we consider the localized proliferation and death process of tumor spheroids.

$$\rho(x) = 70 * \mathbf{1}_{[0.4,0.7]\times[0.4,0.7]}$$

$$\chi_\omega(x) = 25 * \mathbf{1}_{[0.25,0.5]\times[0.25,0.5]}$$

Here $\mathbf{1}(\cdot)$ is the characteristic function. The initial condition is set to be

$$u(0, x, y) = \sin(\pi x)\sin(\pi y)$$

For discretization of the physical domain, we set the uniform mesh size $h_x = h_y = 0.01$. After solving the eigenvalue problem (4.10), there are one positive eigenvalue, which indicates an unstable trajectory. It will lead the uncontrolled dynamics to blow up. In table 4.1 we list several eigenvalues for (4.10). For the stable trajectory $\bar{u}(t, x)$, we take the first negative eigenvalues $\lambda_2 < 0$.

Table 4.1: List of eigenvalues for the eigenvalue problem of tumor growth

λ_1	λ_2	λ_3	λ_4	λ_5
12.1002	-39.6168	-41.0373	-75.9715	-79.0798

We compare the performance of the feedback law with different α, β for a fixed time horizon $T = 1$ with time step $\Delta t = 0.001$ in Table 4.2. Without control ($\alpha = 0, \beta = 0$), we see the tumor density $u(t, x)$ blow up rapidly to the scale of 10^5 at $T = 1$. By the feedback law, say $\alpha = 1, \beta = 1$, the tumor density is decreased to 9.7081, which is a significant improvement comparing before. It can also be observed that, when β term is active, $\|u(T, x)\|_\infty$ is smaller comparing with when $\beta = 0$.

The role of β term is critical for the control of tumor growth. For instance, if $\|u(T, x)\|_\infty = 10$ is the critical value for the tumor density determining whether a patient will die for the tumor or not, then incorporating $\beta = 1$ term in the feedback law will control the tumor density to the safe zone, while $\beta = 0$ cannot.

The left side of Figure 4.1 shows the uncontrolled tumor state at time $T = 1$. We can see the number of tumor $u(t, x)$ blow up rapidly to the scale of 10^5. The right side of Figure 4.1 shows the controlled tumor density with parameters $\alpha = 0.1$, $\beta = 1$. We observe

Table 4.2: The tumor density $\|u(T,x)\|_\infty$ at time $T = 1$ with different pairs of α and β

α	β	$\|u(T,x)\|_\infty$
0	0	27791
1	0	12.8974
1	1	9.7081
0.1	0	4.1642
0.1	1	3.1009

that the tumor density $u(t,x)$ has been decreased significantly by the feedback law. The maximum magnitude at $T = 1$ is 3.1. Figure 4.2 shows the form of feedback control. We see that after $T = 0.6$, the control tends to become a constant, which leads the tumor density to some equilibrium.

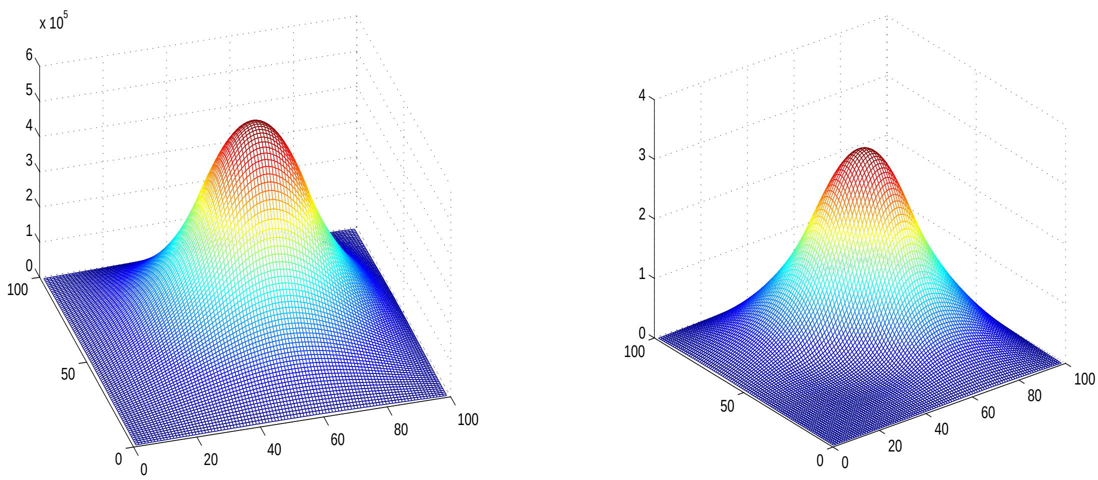

Figure 4.1: The tumor density $u(t,x)$ at time $T = 1$. The left side shows the uncontrolled tumor density, while the right side shows the controlled tumor density with parameters $\alpha = 0.1$, $\beta = 1$.

Our numerics also indicates that the cell production process $\rho(x)$ and the cell degradation process $\chi_\omega(x)$ should have some overlapping region, otherwise the feedback control law fails to suppress the tumor growth. This coincides with the natural philosophy that the drug dose should be applied to affect the region where the tumor grows.

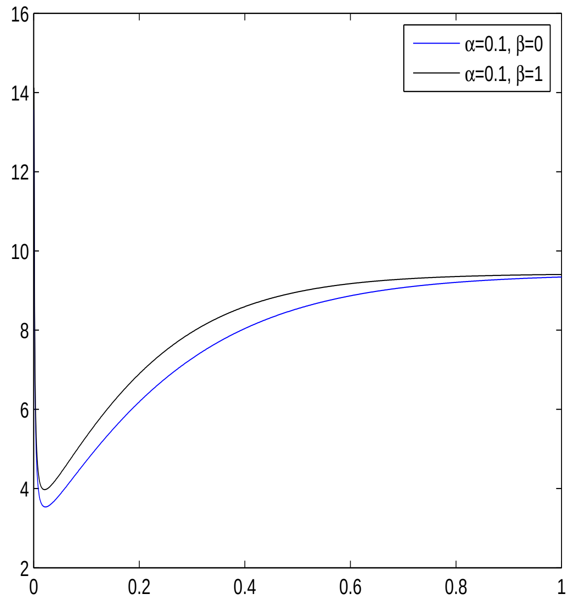

Figure 4.2: The feedback control for tumor growth model

Chapter 5

Stochastic Control on Quantum Spin System

In this chapter, we study a stochastic control problem of quantum spin system under continuous measurement. The objective is to design a feedback control law to global stabilize quantum spin system at the equilibrium states.

5.1 Introduction

Recall from Chapter 1, the state of a quantum system is inherently nondeterministic in nature due to its interaction with external environment. No quantum measurement can give full information on the state of a quantum system. In other words, quantum measurement gives only partial information about the system. Hence, quantum feedback control is complicated comparing to classical feedback control in that it should also consider the back-action of measurement on the system state.

Here we present a typical quantum control scenario, representative of experiments in quantum optics. See Figure 5.1. We wish to control the state of a cloud of atoms, for instance, their angular momentum. To observe the atoms, we scatter a laser probe field off the atoms and measure the scattered light using a homodyne detector. The observation process is then fed into a controller which can feed back a control signal to the atoms through a time-varying magnetic field. Note that, the laser probe interacts with the atoms, hence the observation process can be considered as a noisy observation of the atoms' state.

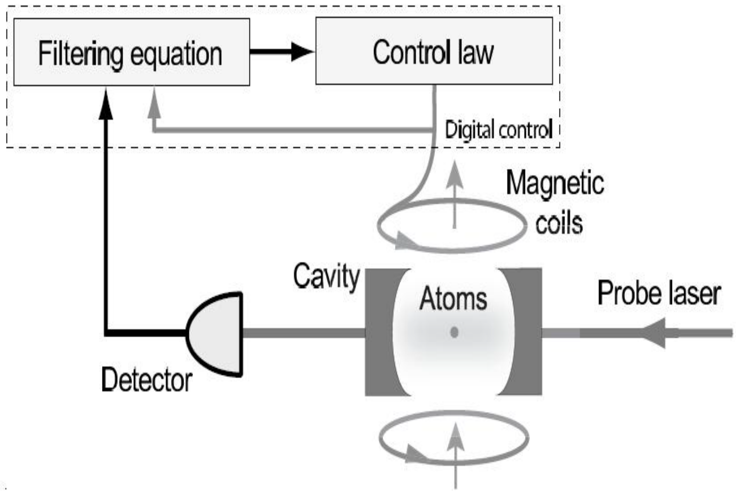

Figure 5.1: A feedback control scenario in quantum optics

The first step in the formulation of quantum feedback control as a stochastic control problem is the development of quantum probability theory. Quantum probability theory can be regarded as the noncommutative counterpart of classical probability theory in the fact that, quantum observables, which are random variables in quantum probability theory, need not commute. Hence the joint distribution of two random variables in quantum probability theory can be defined only if they commute. The physical interpretation of this is that we can only simultaneous measure commuting observables. While in classical probability theory, it is always possible to define the joint distribution of two random variables. By introducing concept of the $*$-algebra (or Von Neumann algebra) $\mathcal{A}$ and quantum probability measure $\mathbb{P}$, the quantum probability space $(\mathcal{A}, \mathbb{P})$ is defined, which is analogous to classical probability space $(\Omega, \mathcal{F}, P)$. The notation of conditional expectation and Bayes rule is also developed for quantum probability theory. Due to the work of Hudson and Parthasarathy [53], stochastic processes for quantum probability and quantum stochastic calculus is developed, which leads to the notion of quantum stochastic differential equations (QSDE).

The next development is the quantum filtering theory by Belvakin in early 1990s [4]. As the state X_t of quantum system is described by a QSDE and the observation process is fixed to be a family of observables $Y_t \in \mathcal{A}$, how to extract the information from the observation process to better describe the quantum system is the objective of the quantum filtering theory. The question is answered by finding the conditional expectation of X_t on the observation process Y_t as a least square estimate. It turns out that this conditional expectation satisfies a classical stochastic differential equation, which is known as the quantum filtering equation. Thus, the quantum feedback control problem is reduced to a classical stochastic control problem for the filter. Based on the foundation of quantum filtering theory, methods from classical nonlinear and stochastic control can be developed and applied to design feedback control law for quantum systems.

To summarize, to design a feedback control on quantum system, it is necessary to separately consider a quantum filtering problem and a state feedback control problem for the filter. In the following section, we will give a brief introduction of the quantum probability theory and quantum filtering theory, then formulate the stabilization problem of quantum spin system. A feedback control law with switching term is designed to global stabilization the spin system at an eigenstate by continuous inputs. Numerical results are demonstrated.

5.2 Quantum Probability and Quantum Filtering Theory

5.2.1 Quantum Probability Theory

The source of inspiration for doing quantum probability lies in the methods by the physicists to compute probabilities of events concerning the subatomic world of elementary particles. These methods lead to a generalization of classical probability theory.

Quantum probability theory is the noncommutative counterpart of classical probability theory. In quantum probability theory, the random variables are observables, which are self-adjoint operators on a Hilbert space. Observables may not commute and the product of two observables may not be observable also unless they commute. This is the key difference form the classical probability theory. The fact can be seen in a simple example from the spin-$\frac{1}{2}$ system. Recall from 1.1, the Pauli matrices σ_x, σ_y, σ_z given by (1.4) are the observables, which represent spin measurement in the x, y, z direction. It is easy to verify that $\sigma_x \sigma_y = i\sigma_z$, $\sigma_y \sigma_x = -i\sigma_z$. That is, σ_x and σ_y do not commute.

Recall that an observable X has spectral decomposition, $X = \sum_{a \in spec(X)} aP_a$. The projection operator P_a can be regarded as the event that the random variable X takes the values a. In order to measure the quantities associated with observable, a state is represented by a density matrix ρ, which belongs to the set

$$S = \{\rho \in \mathcal{C}^{N\times N} : \rho^* = \rho, \rho \geq 0, Tr(\rho) = 1\} \tag{5.1}$$

This is the noncommutative counterpart of probability density function. In this setting, the probability of the event P_a can be measured by $Tr(\rho P_a)$. In particular, the expectation of an observable X is given by $Tr(\rho X)$.

Analogous to σ-algebra in classical probability space, a $*$-algebra $\mathscr{N}$ on a Hilbert space $\mathscr{H}$ is a set of operators which is closed under linear combination, product and adjoint of operators in $\mathscr{N}$. A linear map $\mathbb{P} : \mathscr{N} \to \mathbb{R}$ that is positive ($\mathbb{P}(A) \geq 0$ if $A \geq 0$) and normalized ($\mathbb{P}(\mathrm{I}) = 1$) is called a state on $\mathscr{N}$, which can be regarded as a probability measure. It is clear that we can always define the state as

$$\mathbb{P}(X) = Tr(\rho X)$$

for some density matrix ρ.

The pair $(\mathscr{N}, \mathbb{P})$ consists of a quantum probability space.

By the following spectral theorem, we will see that the classical probability theory is the commutative counterpart of quantum probability theory.

Theorem 5.2.1 (Spectral Theorem) *Let $\mathscr{A}$ be a* commutative *$*$-subalgebra in $\mathscr{N}$ on a finite-dimensional Hilbert space $\mathscr{H}$, and let $\mathbb{P}$ is a state on $\mathscr{A}$. Then there is a probability space $(\Omega, \mathcal{F}, \mathbf{P})$, and a map ι from $\mathscr{A}$ onto the set of measurable functions on Ω that is a $*$-isomorphism,i.e. a linear bijection with $\iota(AB) = \iota(A)\iota(B)$ and $\iota(A^*) = \iota(A)^*$, and moreover,*

$$\mathbb{P} = E_{\mathbf{P}}(\iota(A))$$

Proof: Since the Hilbert space $\mathscr{H}$ is of finite dimension, without loss of generality we can assume $\mathscr{H} = \mathbf{C}^n$ and $\mathscr{A}$ is a commutative $*$-algebra of $n \times n$ matrices. As every elements in $\mathscr{A}$ commutes, there exists a unitary matrix U such that U^*AU is a diagonal matrix for every $A \in \mathscr{A}$. Let $\Omega = \{1, \ldots, n\}$, define $\iota(A)$: $\Omega \to \mathbf{C}$ by $\iota(A)(i) = (U^*AU)_{ii}$ for every $A \in \mathscr{A}$. Next, define $\mathcal{F} = \sigma\{\iota(A) : A \in \mathscr{A}\}$. Finally, define $\mathbf{P}(S) = \mathbb{P}(\iota^{-1}(\chi_s))$ for every $S \in \mathcal{F}$. We construct $(\Omega, \mathcal{F}, \mathbf{P})$ and ι explicitly.

Next we introduce the notion of conditional expectation for quantum probability theory. Remember that, we can only define the joint distribution of two commuting events in quantum probability. Hence only conditional expectation for commutative subalgebra in a quantum probability space can be defined.

Definition 5.2.1 (Conditional expectation) *Let $(\mathscr{N}, \mathbb{P})$ be a finite-dimensional quantum probability space and let $\mathscr{A} \subset \mathscr{N}$ be a commutative $*$-subalgebra. Let*

$$\mathscr{A}' = \{B \in \mathscr{N} : AB = BA, \forall A \in \mathscr{A}\}$$

be the commutant of $\mathscr{A}$. Then $\mathbb{P}(\cdot|\mathscr{A}) : \mathscr{A}' \to \mathcal{A}$ is called the conditional expectation from $\mathscr{A}'$ onto $\mathscr{A}$ if

$$\mathbb{P}(\mathbb{P}(B|\mathscr{A})A) = \mathbb{P}(BA)$$

for all $A \in \mathscr{A}$, $B \in \mathscr{A}'$.

It's important to be aware that $\mathbb{P}(B|\mathscr{A})$ is the least mean square estimate of B in $\mathscr{A}$. In case of $\mathscr{A}$ as the $*$-algebra generated by the observation process, then the conditional expectation $\mathbb{P}(B|\mathscr{A})$ gives the best estimate of observable B in least square sense.

If we can find an orthogonal basis for $\mathscr{A}$, say $\mathscr{A}$ =span$\{P_a\}$ for some set of projections P_a, then it is easy to obtain an explicit expression for $\mathbb{P}(B|\mathscr{A})$,

$$\mathbb{P}(B|\mathscr{A}) = \sum_{P \in \{P_a\}} \frac{\mathbb{P}(PB)}{\mathbb{P}(P)} P$$

For example, Let $\mathscr{H} = \mathbf{C}^3$, $\mathscr{N} = M_3$, i.e., space of 3×2 complex matrices, and the state $\mathbb{P}(X) =< \psi, X\psi >$ with $\psi = (1\,1\,1)^T/\sqrt{3}$, define

$$A = \begin{pmatrix} 4 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 5 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

Let $\mathscr{A}$ be the $*$-algebra generated by A, then

$$\mathbb{P}(B|\mathscr{A}) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix} \quad \in \mathscr{A}$$

5.2.2 Stochastic Processes on Quantum Probability Space

In this section, we introduce the stochastic processes in quantum probability space. They are quantum analogies of classical stochastic processes, for instance, families of Poisson and Wiener processes.

We start with introducing some notation about the tensor products of Hilbert spaces. Let $\mathscr{H}_i$, $i = 1, 2, \ldots, n$ be Hilbert spaces, we write

$$\mathscr{H} = \mathscr{H}_1 \otimes \mathscr{H}_2 \otimes \ldots \otimes \mathscr{H}_n = \bigotimes_{i=1}^{n} \mathscr{H}_i \tag{5.2}$$

$$\lambda_(u) = u_1 \otimes u_2 \otimes \ldots \otimes u_n = \bigotimes_{i=1}^{n} u_i \tag{5.3}$$

$\mathscr{H}$ is called a tensor product of $\mathscr{H}_i$, $\lambda(u)$ is called the tensor product of the vectors $u_i \in \mathscr{H}_i$. If $\mathscr{H}_i = h$ for all i, then $\mathscr{H}$ is called the n-fold tensor product of h and denoted by $h^{\otimes n}$. If $u_i = u$ for all i, then $\lambda(u)$ is denoted by $u^{\otimes n}$ and called the n-th power of u.

Let S_n denote the group of all permutation of the set $1, 2, \ldots, n$. For each $\sigma \in S_n$ let U_σ be defined on the product vectors in $\mathscr{H}^{\otimes n}$ by

$$U_\sigma u_1 \otimes u_2 \otimes \ldots \otimes u_n = u_{\sigma^{-1}(1)} \otimes \ldots \otimes u_{\sigma^{-1}(n)} \tag{5.4}$$

define the closed subspace

$$\mathscr{H}^{\otimes_s n} = \{u \in \mathscr{H}^{\otimes n} | U_\sigma u = u \text{ for all} \sigma \in S_n\} \tag{5.5}$$

called the n-fold symmetric tensor products of $\mathscr{H}$. When $n = 0$, the 0-fold product is the one dimensional complex plane $\mathbf{C}$ and 1-fold product is $\mathscr{H}$ itself.

Next we will define the stochastic process on Fock spaces. The symmetric Fock space over a Hilbert space $\mathscr{H}$ is defined as

$$\mathcal{F}_s(\mathscr{H}) = \bigoplus_{n=0}^{\infty} \mathscr{H}^{\otimes_s n} \tag{5.6}$$

For every $g \in \mathscr{H}$, the element $e(g) \in \mathcal{F}_s(\mathscr{H})$

$$e(g) = \bigoplus_{n=0}^{\infty} (n!)^{-1/2} g^{\otimes n} \tag{5.7}$$

is called the exponential vector associated with g. for any $f, g \in \mathscr{H}$,

$$< e(f), e(g) >= exp(< f, g >)$$

It's easy to see that the set $\{e(g)|g \in \mathscr{H}\}$ of all exponential vectors is linearly independent and total in $\mathcal{F}_s(\mathscr{H})$. Hence the linear span of all exponential vectors $D = \{\alpha e(g)|\alpha \in \mathcal{C}, g \in \mathscr{H}\}$ is a dense subspace of $\mathcal{F}_s(\mathscr{H})$. Consider the action induced on D by the map $e(g) \to e(Ug + f)$ where U denotes a unitary operator on $\mathscr{H}$. This is not inner product preserving. Indeed, for any $g_1, g_2 \in \mathscr{H}$,

$$< e(Ug_1 + f), e(Ug_2 + f) >=< e(g_1), e(g_2) > exp\{||f||^2 + < Ug_1, f > + < f, Ug_2 >\}$$

This shows that the map

$$e(g) \to \{exp(-||f||^2 - < f, Ug >)\}e(Ug + f)$$

yields an isometry of D onto itself. Hence these exists a unique unitary operator $W(f)$ in $\mathcal{F}_s(\mathscr{H})$

$$W(f, U)e(g) = \{exp(-||f||^2 - < f, Ug >)\}e(Ug + f), \quad f, g \in \mathscr{H} \tag{5.8}$$

called the Weyl operators with the pair (f, U).

In particular, we get the following relation

$$W(f) = W(f, 1), \quad \Gamma(U) = W(0, U) \tag{5.9}$$

for f in $\mathscr{H}$ and U being a unitary operator on $\mathscr{H}$.

Consider the unitary parameter group $W(tf)_{t\in\mathbb{R}}$, it is continuous in strong operator topology. Hence by Stone's theorem there exists a self-adjoint operator $B(f)$ such that

$$W(tf) = exp(itB(f))$$

The operator $B(f)$ is called field operator.

The operator $\Gamma(U)$ is called the second quantization of U. Since $\Gamma(U)\Gamma(V) = \Gamma(UV)$, so for every one parameter unitary group $U_t = e^{itH}$ in $\mathscr{H}$ there corresponds a one parameter unitary group $\{\Gamma(U_t)|t \in \mathbb{R}\}$ in $\mathcal{F}_s(\mathscr{H})$. By Stone's theorem again, these exists a self-adjoint operator Λ_t such that

$$\Gamma(e^{itH}) = exp(it\Lambda_t)$$

The operator Λ_t is interpreted as the observable to counts how many particles are present in the interval $[0, t)$. It's the counterpart of poisson process in classical probability theory.

Consider the operator process $\{B_t^\varphi = B(e^{i\varphi}\chi_{[0,t]}) : t \in [0, T]\}$ for $\varphi \in \mathscr{H}$. B_t^φ and B_s^ψ commutes for all $s, t \in [0, T]$, hence the $*$-algebra generated by $\{B_t^\varphi$ is commutative. By Spectral Theorem, there exist a $*$-isomorphism ι such that $\iota(B_t^\varphi)$ is a classical random variable on classical probability space $(\Omega^\varphi, \mathcal{F}^\varphi, \mathbf{P}^\varphi)$. By calculating the characteristic function of $B(f)$, we get $B(f)$ is a Gaussian random variable. Hence $\iota(B_t^\varphi)$ has independent increments and $\iota(B_t^\varphi) - \iota(B_s^\varphi)$ is a mean zero Gaussian random variable. More precisely, we get $\iota(B_t^\varphi)$ is a Wiener process.

Finally we define the annihilation operator A_t and creation operator A_t^* by

$$A_t = \frac{1}{2}(B(i\chi_{[0,t)}) - iB(\chi_{[0,t)})) \tag{5.10}$$

$$A_t^* = \frac{1}{2}(B(i\chi_{[0,t)}) + iB(\chi_{[0,t)})) \tag{5.11}$$

They can be regarded as Wiener process in quantum probability space with the properties that A_t and A_t^* do not commute with each other.

5.2.3 Quantum Stochastic Calculus

In classical probability theory, by using Ito's isometry, the stochastic Ito's integral can be defined as the L^2 limit of the integration on simply functions, see [52]. Similar approach is applied to define quantum stochastic integral. But the difference is that the quantum stochastic integral are driven simultaneously by the noncommutative forces A_t and A_t^*, and even Λ_t. In 1980's, Hudson and Parthasarathy [53] developed the quantum stochastic calculus and extended the Ito's rule of classical probability theory.

We are interested to define the stochastic calculus against the processes Γ_t, A_t and A_t^*, which are known as the fundamental noises. Let M_t be one of the above three processes. We want to define the integral

$$\int_0^t L_s dM_s \tag{5.12}$$

Given a Hilbert space $\mathscr{H} = L^2([0, T])$, we can define a symmetric Fock space $\mathcal{F} = \mathcal{F}_s(\mathscr{H})$ by equation (5.6). On the interval $[0, T]$, we introduce the notation $\mathcal{F}_{t]}$, $\mathcal{F}_{[t}$, $\mathcal{F}_{[s,t]}$ to denote the restriction of $\mathcal{F}$ on the interval $[0, t]$, $[t, T]$, $[s, t]$. It follows that

$$\mathcal{F} = \mathcal{F}_{s]} \otimes \mathcal{F}_{[s,t]} \otimes \mathcal{F}_{[t} \quad 0 < s < t < T \tag{5.13}$$

From equation (5.7), we can define the Weyl operator on $\mathcal{F}_s(\mathscr{H})$. Let $\mathscr{W} = \mathscr{B}(\mathcal{F}_s(\mathscr{H}))$, that is, the $*$-algebra generated by all the operators on $\mathcal{F}_s(\mathscr{H})$. We can split the algebra $\mathscr{W}$ as follows

$$\mathscr{W} = \mathscr{W}_{s]} \otimes \mathscr{W}_{[s,t]} \otimes \mathscr{W}_{[t} = \mathscr{B}(\mathcal{F}_{s]}) \otimes \mathscr{B}(\mathcal{F}_{[s,t]}) \otimes \mathscr{B}(\mathcal{F}_{[t}) \tag{5.14}$$

A process of operators $\{L_t\}$ is adapted to $\mathscr{W}$ if L_t is affiliated to $\mathscr{W}_{t]}$ for every t.

Let $\{t_i | i = 0, 1, \ldots n, t_i < t_{i+1}\}$ be a partition of interval $[0, T]$ with $t_0 = 0$, $t_n = T$. We construct the simple process

$$L_t = \sum_{i=0}^{n-1} L_{t_i} \chi_{[t_i, t_{i+1})}(t) \tag{5.15}$$

the stochastic integral for simple process can defined as

$$\int_0^t L_s dM_s = \sum_{i=0}^{n-1} L_{t_i}(M_{t_{i+1}\wedge t} - M_{t_i \wedge t}) \tag{5.16}$$

In general, for an adapted operator process L_t, we can define the stochastic integral $\int_0^t L_s dM_s$ as the limit of integral of simple process, similar to classical construction. An equivalent for to write the stochastic integral is to write

$$dX_t = L_t dM_t$$

Hudson and Parthasarathy give the following theorem which extends the Ito's rule of classical probability theory.

Theorem 5.2.2 (Quantum Ito's Rule) *Let X_t and Y_t be well defined stochastic integrals in the form of*

$$dX_t = B_t d\Lambda_t + C_t dA_t + D_t dA_t^* + E_t dt \tag{5.17}$$

for some adapted process B_t, C_t, D_t, E_t. Then the product $X_t Y_t$ is well defined stochastic integral and satisfies

$$d(X_t Y_t) = X_t dY_t + Y_t dX_t + dX_t dY_t \tag{5.18}$$

$dX_t dY_t$ is evaluated according to the quantum Ito table

$dX \setminus dY$	dA_t	$d\Lambda_t$	dA_t^*	dt
dA_t	0	dA_t	dt	0
$d\Lambda_t$	0	$d\Lambda_t$	dA_t^*	0
dA_t^*	0	0	0	0
dt	0	0	0	0

The Quantum Ito's Rule gives us the covariance structure for the process Γ_t, A_t and A_t^*. Because Γ_t, A_t and A_t^* do not commute with each other, we see that the covariance matrix is not symmetric.

5.2.4 Quantum Filtering Theory

In this section, we focus on describing the quantum filtering theory for quantum optics model.

Recall from Section 2.1, we can describe the evolution of a quantum system in a unitary fashion. Let U_t be a unitary operator which satisfies the Schrödinger type quantum stochastic differential equation (QSDE)

$$dU_t = (LdA_t^* - L^*dA_t - \frac{1}{2}L^*Ldt - iHdt)U_t, \quad U_0 = I \tag{5.19}$$

where A_t, A_t^* are the noncommuting white noise processes defined in (5.10) (5.11), H is the Hamiltonian and L is an atomic(dipole) operator, which is also called Lindblad operator. The adjoint operator U_t^* satisfies

$$dU_t^* = U_t^*(L^*dA_t - LdA_t^* - \frac{1}{2}L^*Ldt + iHdt), \quad U_0^* = I \tag{5.20}$$

The operator U_t gives the evolution of the observable X. The observation of X at time t is described by the observable $X_t = U_t^*XU_t$. Here we use the notation $X_t = j_t(X)$ to denote the evolution of X at time t. By using Quantum Ito's rule, we get

$$\begin{aligned} dX_t = dj_t(X) =& U_t^*d(XU) + d(U_t^*X)U + d(U_t^*)Xd(U) \\ =& U_t^*X(LdA_t^* - L^*dA_t - \frac{1}{2}L^*Ldt - iHdt)U_t \\ &+ U_t^*(L^*dA_t - LdA_t^* - \frac{1}{2}L^*Ldt + iHdt)XU_t + U_t^*L^*XLU_t \end{aligned}$$

combine the common term, and using the notation of Lie bracket $[H, X] = HX - XH$, we get

$$dX_t = j_t(\mathcal{L}_{L,H}(X))dt + j_t([L^*, X])dA_t + j_t([X, L])dA_t^* \tag{5.21}$$

where the (Lindblad) generator given by

$$\mathcal{L}_{L,H}(X) = i[H, X] + L^*XL - \frac{1}{2}(XL^*L + L^*LX) \tag{5.22}$$

Through the above derivation, we have described the evolution of the quantum system and its interaction with the outer optical field. Now we turn to the measurement of the system. Recall that, only commuting events can be measured simultaneously in experiment. Hence it is essential that the observation process $\{Y_t\}$ must commute with itself at different time. This is called *self-nondemolition property.* In general, there are two types of measurement which are commonly used in quantum optics:

- direct photodetection(photon counting) where the observation at time t is given by $Y_t^\Lambda = U_t^* \Lambda_t U_t$
- homodyne detection given by $Y_t^W = U_t^*(A_t + A_t^*)U_t$

by using quantum Ito's rule, and note that the Lindblad operator L commutes with Λ_t, A_t and A_t^*, we have the following derivation

$$\begin{aligned}
dY_t^\Lambda &= dU_t^*(\Lambda_t U_t) + U_t^* d(\Lambda_t U_t) + dU_t^* d(\Lambda_t U_t) \\
&= dU_t^*(\Lambda_t U_t) + U_t^*(d\Lambda_t U_t + \Lambda_t dU_t + d\Lambda_t dU_t) + dU_t^*(d\Lambda_t U_t + \Lambda_t dU_t + d\Lambda_t dU_t) \\
&= U_t^*(L^* dA_t - L dA_t^* - \frac{1}{2}L^* L dt + iH dt)\Lambda_t U_t + d\Lambda_t \\
&\quad + U_t^* \Lambda_t (L dA_t^* - L^* dA_t - \frac{1}{2}L^* L dt - iH dt)U_t + U_t^* L U_t dA_t^* \\
&\quad + U_t^* L^* U_t dA_t + U_t^* L^* \Lambda_t L U_t dt + U_t^* L^* L U dt \\
&= d\Lambda_t + U_t^* L^* U_t dA_t + U_t^* L U_t dA_t^* + U_t^* L^* L U dt
\end{aligned}$$

$$\begin{aligned}
dY_t^W &= dU_t^*(A_t + A_t^*)U_t + U_t^* d[(A_t + A_t^*)U_t)] + dU_t^* d[(A_t + A_t^*)U_t)] \\
&= dU_t^*(A_t + A_t^*)U_t + U_t^*[(dA_t + dA_t^*)U_t + (A_t + A_t^*)dU_t + (dA_t + dA_t^*)dU_t)] \\
&\quad + dU_t^*[(dA_t + dA_t^*)U_t + (A_t + A_t^*)dU_t + (dA_t + dA_t^*)dU_t)] \\
&= U_t^*(L^* dA_t - L dA_t^* - \frac{1}{2}L^* L dt + iH dt)(A_t + A_t^*)U_t + dA_t + dA_t^* \\
&\quad + U_t^*(A_t + A_t^*)(L dA_t^* - L^* dA_t - \frac{1}{2}L^* L dt - iH dt)U_t + U_t^* L U_t dt \\
&\quad + U_t^* L^* U_t dt + U_t^* L^*(A_t + A_t^*)L U_t dt \\
&= U_t^*(L + L^*)U_t dt + dA_t + dA_t^*
\end{aligned}$$

So we obtain

$$dY_t^\Lambda = d\Lambda_t + U_t^* L^* U_t dA_t + U_t^* L U_t dA_t^* + U_t^* L^* L U dt \tag{5.23}$$

$$dY_t^W = U_t^*(L+L^*)U_t dt + dA_t + dA_t^* \tag{5.24}$$

Given the observation process Y_s satisfying (5.23) or (5.24) for $0 \le s \le t$, what is the best estimation of $\hat{X}_t$ of the observable X_t of the system (5.21) based on these observations? This is the objective of the quantum filtering problem.

From standard theory, the conditional expectation

$$\hat{X}_t = \pi_t(X) = \mathbb{P}(X_t|\mathscr{Y}_t) \tag{5.25}$$

where $\mathscr{Y}_t = \mathscr{B}(Y_s : 0 \le s \le t)$, is the least mean square estimate for observable X_t. In the following, we will derive the stochastic differential equation for $\pi_t(X)$. It turns out this is a classical stochastic differential equation driving by the Wiener process.

Recall that, we can only define the conditional expectation $\hat{X}_t$ only if X_t is in the commutant of $\mathscr{Y}_t$. Actually this is fulfilled since the observation process Y_t is measured through direct photodection or homodyne detection. By the self-nondemolition property, it can be shown X_t commutes with $\mathscr{Y}_t$. That is,

$$[X_t, Y_s] = 0, \quad \forall\ s \le t \tag{5.26}$$

Now we state the the **quantum filtering equation** in case of homodyne detection, the proof will be shown later. The conditional expectation $\pi_t(X)$ satisfies

$$d\pi_t(X) = \pi_t(\mathcal{L}_{L,H}(X))dt + [\pi_t(L^*X + XL) - \pi_t(L^*+L)\pi_t(X)](dY_t - \pi_t(L^*+L)dt) \tag{5.27}$$

In case of finite dimension Hilbert space, write $\pi_t(X) = Tr(\rho_t X)$ for some conditional density matrix ρ_t,

$$Tr(\frac{d\rho_t}{dt}X) = Tr(\rho_t\mathcal{L}_{L,H}(X)dt) + \{Tr(\rho_t(L^*X + XL)) - Tr(\rho_t(L^*+L))Tr(\rho_t X)\}dW_t$$

$$\frac{d\rho_t}{dt}X = \rho_t\mathcal{L}_{L,H}(X)dt + \{\rho_t L^* + L\rho_t - Tr(\rho_t(L^*+L))\rho_t\}XdW_t$$

Note that

$$\rho_t\mathcal{L}_{L,H}(X) = \mathcal{L}_{L,H}^*(\rho_t)X$$

hence we obtain explicitly the QSDE for ρ_t,

$$d\rho_t = (-i[H,\rho_t] + L\rho_t L^* - \frac{1}{2}\rho_t L^*L - \frac{1}{2}L^*L\rho_t)dt + (L\rho_t + \rho_t L^* - Tr(\rho_t(L+L^*))\rho_t)dW_t \tag{5.28}$$

$$= \mathcal{L}_{L,H}^*(\rho_t) + (L\rho_t + \rho_t L^* - Tr(\rho_t(L+L^*))\rho_t)dW_t \tag{5.29}$$

where $dW_t = dY_t - Tr((L^* + L)\rho_t)dt$. In the following, we will prove the quantum filtering equation (5.28) by innovation method and see that the process W_t is actually a Wiener process. The procedure follows the classical treatment on nonlinear filtering [40]. We see that the quantum filtering equation is a quantum analog of the classical Kushner-Stratonovich equation of nonlinear filtering. The proof is briefly stated as follows:

Step 1: define $h_s = j_s(L + L^*)$, $\hat{h}_s = \mathbb{P}(h_s|\mathscr{Y}_s) = \pi_s(L + L^*)$, Note

$$dY_t = h_t dt + dZ_t, \quad \text{where} \quad dZ_t = dA_t + dA_t^*$$

then

$$I_t = Y_t - \int_0^t \hat{h}_s ds$$

is a $\mathscr{Y}_t$-adapted Weiner process.

Step 2: Note

$$dX_t = \beta_t dt + dm_t$$

where $dm_t = \lambda_t dA_t + \mu_t dA_t^*$, then the process

$$M_t = \hat{X}_t - \hat{X}_0 - \int_0^t \hat{\beta}_s ds$$

is a $\mathscr{Y}_t$ martingale. By martingale representation theorem. we have

$$M_t = \int_0^t \gamma_s dI_s$$

for some adapted process $\gamma_t \in \mathscr{Y}_t$.

Step 3: We obtain two expression for $\widehat{X_t Y_t}$:

$$d\widehat{X_t Y_t} = (\widehat{\beta_t Y_t} + \widehat{X_t h_t} + \hat{\lambda}_t)dt + dM_1(t)$$

where $M_1(t)$ is a $\mathscr{Y}_t$ martingale. And

$$d(\hat{X}_t Y_t) = (\hat{\beta}_t Y_t + \hat{X}_t \hat{h_t} + \gamma_t)dt + (\gamma_t Y_t + \hat{X}_t)dI_t$$

Note that $\widehat{X_t Y_t} = \hat{X}_t Y_t$, by uniqueness,

$$\widehat{\beta_t Y_t} + \widehat{X_t h_t} + \hat{\lambda}_t = \hat{\beta}_t Y_t + \hat{X}_t \hat{h_t} + \gamma_t$$

Therefore,

$$\gamma_t = \widehat{X_t h_t} + \hat{\lambda}_t - \hat{X}_t \hat{h_t}$$

Hence, the filtering equation (5.27) can be derived.

5.3 Quantum Feedback Control

In this section, we formulate the stochastic control problem of quantum spin system under continuous measurement. As shown in Figure 5.1, a typical quantum control experiment in quantum optics is to control the angular momentum of a cloud of atoms. To observe the atoms, a laser probe field is scattered off the atoms, then the scattered light is measured using a homodyne detector. The observation process is fed into a controller which can feed back a control signal to the atoms through a time-varying magnetic field.

In case of a quantum spin system with fixed angular momentum J ($2J \in \mathbb{N}$), the dimension of the Hilbert space $X = \mathbb{C}^N$ is $N = 2J + 1$. When we observe the angular moment on z-axis and apply the magnetic field along y-axis, the corresponding quantum filtering equation (5.28) is in the form of

$$d\rho_t = -iu_t[F_y, \rho_t]dt - \frac{1}{2}[F_z, [F_z, \rho_t]]dt + \sqrt{\eta}(F_z\rho_t + \rho_t F_z - 2Tr(F_z\rho_t)\rho_t)dW_t \tag{5.30}$$

$$dy_t = 2\sqrt{\eta}Tr(F_z\rho_t)dt + dW_t \tag{5.31}$$

where $0 < \eta \leq 1$ is the detector efficiency, $u_t \in \mathbb{R}$ is the control input, F_y and F_z are self-adjoint angular moment operators along x and y axis of the form

$$F_y = \frac{1}{2i}\begin{pmatrix} 0 & -c_1 & & & \\ c_1 & 0 & -c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & c_{2J-1} & 0 & -c_{2J} \\ & & & c_{2J} & 0 \end{pmatrix}, c_m = \sqrt{(2J+1-m)m}$$

$$F_z = \begin{pmatrix} J & & & & \\ & J-1 & & & \\ & & \ddots & & \\ & & & -J+1 & \\ & & & & -J \end{pmatrix}$$

Comparing to (5.28), we see the Hamiltonian $H = u_t F_y$ and the Lindblad operator $L = F_z$. Recall that $\rho_t \in S$ where

$$S = \{\rho \in \mathcal{C}^{N\times N} : \rho^* = \rho, \rho \geq 0, Tr(\rho) = 1\}$$

Let $\{\Psi_i : i = 0 \dots 2J\}$ be the standard basis in $\mathbf{C}^N$, that is, Ψ_i is the vector with 1 at its ith component, 0 otherwise. The state $\rho_{\Psi_i} = \Psi_i \Psi_i^*$ is called an eigenstate of the quantum spin system.

Let us first explore the dynamical behavior of equation (5.30) in deterministic case $(\eta = 0)$.

Diagonal invariant: consider the case

$$d\rho_t = -\frac{1}{2}[F_z, [F_z, \rho_t]]dt$$

then $\rho_t \to diag(\rho_0)$ as $t \to \infty$.

Proof: F_z is a diagonal matrix with $diag(a_1, \dots, a_N)$, $a_k = J + 1 - k$, $k = 1 \dots N$. It is easy to see that for the (i, j) entry of ρ_t, it satisfies

$$d\rho_{ij} = -\frac{1}{2}(a_i - a_j)^2 \rho_{ij} dt$$

For $i \neq j$, ρ_{ij} is exponentially decaying to 0; for $i = j$, $\rho(t)_{ii} = \rho(0)_{ii}$. $\Box$

Equally distributed: consider the case

$$d\rho_t = -iu_t[F_y, \rho_t]dt - \frac{1}{2}[F_z, [F_z, \rho_t]]dt$$

For any constant control $u_t \neq 0$, $\rho_t \to diag(\frac{1}{N}, \dots, \frac{1}{N})$ as $t \to \infty$ where $N = 2J + 1$.

When the detector coefficient η is active, through the following theorem, we see that without controlling, ρ_t will converge almost surely to one of eigenstates as $t \to \infty$.

Theorem 5.3.1 (Quantum state reduction) *For any $\rho_0 \in S$, the solution ρ_t with $u_t = 0$ converges a.s as $t \to \infty$ to one of $\rho_{\Psi_m} = \Psi_m \Psi_m^*$, that is*

$$\rho_t \to \rho_{\Psi_m} \quad a.s., \quad t \to \infty$$

and

$$E\rho_t \to diag(\rho_0), \quad t \to \infty$$

So,

$$Pr(\lim_{t\to\infty} \rho_t = \rho_{\Psi_m}) = (\rho_0)_{mm} = Tr(\rho_0 \rho_{\Psi_m})$$

Proof: When $u_t = 0$, consider the Lyapunov function $v(\rho) = Tr(F_z^2\rho) - (Tr(F_z))$. After calculation, we find the generator $\mathscr{A} v(\rho) = -4\eta\, v(\rho)^2 \leq 0$, hence

$$Ev(\rho_t) = v(\rho_0) - 4\eta \int_0^t Ev(\rho_s)^2\, ds$$

by using Ito's rules. As $v(\rho) \geq 0$,

$$4\eta \int_0^t Ev(\rho_s)^2\, ds = v(\rho_0) - Ev(\rho_t) \leq v(\rho_0) < \infty$$

By monotone convergence theorem, we have

$$\int_0^\infty v(\rho_s)^2\, ds < \infty \quad a.s$$

As the limit of $v(\rho_t)$ as $t \to \infty$ exist a.s. by the Lyapunov theorem, we have $v(\rho_t) \to 0$ a.s. But the only states ρ that satisfy $v(\rho) = 0$ are $\rho = \Psi_m \Psi_m^*$.

From (5.30), we have

$$\rho_t = \int_0^t -\frac{1}{2}[F_z, [F_z, \rho_t]]\, dt + \int_0^t \sqrt{\eta}(F_z\rho_t + \rho_t F_z - 2Tr[F_z\rho_t]\rho_t)\, dW_t$$

then $E\rho_t = \int_0^t -\frac{1}{2}[F_z, [F_z, E\rho_t]]\, dt$. By the diagonal invariant property, $E\rho_t \to diag(\rho_0)$, as $t \to \infty$. Since $\lim\limits_{t\to\infty} E\rho_t = \sum \rho_{\Psi_m} Pr(\lim\limits_{t\to\infty} \rho_t = \rho_{\Psi_m})$, so

$$Pr(\lim_{t\to\infty} \rho_t = \rho_{\Psi_m}) = (\rho_0)_{mm} = Tr(\rho_0 \rho_{\Psi_m}) \quad \square$$

By Theorem 5.3.1, we see that without control, the convergence of ρ_t to a eigenstate is random. Hence the control problem for quantum spin system is to find a control input u_t in such way to globally converge the quantum state ρ_t to some desired eigenstate ρ_{Ψ_i}. This is a stochastic stability problem.

We define the stochastic stability according to [39]. The equilibrium ρ_f is said to be stable in probability if

$$\lim_{\rho_0 \to \rho_f} Pr(\sup_{0<t<\infty} ||\rho_t - \rho_f|| \geq \epsilon) = 0 \quad \forall \epsilon > 0 \tag{5.32}$$

the equilibrium ρ_f is globally stable if it is stable in probability and additionally

$$Pr(\lim_{t\to\infty} \rho_t = \rho_f) = 1 \tag{5.33}$$

Here we introduce three performance functionals which have the properties: $0 \leq V_{\rho_f}(\rho) \leq 1$ and $V_{\rho_f}(\rho) = 0$ if and only if $\rho = \rho_f$.

$$V^I_{\rho_f} = 1 - Tr(\rho\rho_f) \tag{5.34}$$

$$V^{II}_{\rho_f} = 1 - (Tr(\rho\rho_f))^2 \tag{5.35}$$

$$V^{III}_{\rho_f} = Tr(F_z^2 \frac{\rho + \rho_f}{2}) - (Tr(F_z \frac{\rho + \rho_f}{2}))^2 \tag{5.36}$$

In order to study stochastic stability, the stochastic version of Lyapunov stability theory and LaSalles' invariance theorem are important tools to use. Next we state the following stochastic version of the Lyapunov theorem. Assume $V(\cdot)$ is a nonnegative real-valued continuous function on S, and define $\rho_t^z = \rho_t$ such that $\rho_0 = z$. For $\epsilon > 0$, let $Q_\epsilon = \{\rho \in S : V(\rho) < \epsilon\}$, a stop time $\tau_\epsilon = \inf\{t : \rho_t^z \notin Q_\epsilon\}$ and $\tilde{\rho}_t^z = \rho^z_{t\wedge\tau_\epsilon}$. Let $\mathscr{A}_\epsilon$ be the weak infinitesimal operator on $\tilde{\rho}_t^z$, then we get the following theorem.

Theorem 5.3.2 (Lyapunov theorem) *If $\mathscr{A}_\epsilon V \leq 0$ in Q_ϵ. Then the followings hold:*

1. $\lim_{t\to\infty} V(\tilde{\rho}_t^z)$ *exists a.s., so $V(\rho_t^z)$ converges for a.e. path remaining in Q_ϵ.*

2. $Pr(\lim_{t\to\infty} \mathscr{A}_\epsilon V(\tilde{\rho}_t^z)) = 0$, *so $\mathscr{A}_\epsilon V(\rho_t^z)) \to 0$ in probability as $t \to \infty$ for almost all paths which never leave Q_ϵ.*

3. *for $z \in Q_\epsilon$ and $\alpha \leq \epsilon$ we have the uniform estimate*

$$Pr(\sup_{0\leq t<\infty} V(\rho_t^z) \geq \alpha) = Pr(\sup_{0\leq t<\infty} V(\tilde{\rho}_t^z) \geq \alpha) \leq \frac{V(z)}{\alpha} \tag{5.37}$$

4. *If $V(\tilde{z}) = 0$ and $V(\rho) \neq 0$ for $\rho \neq \tilde{z}$, then $\tilde{z}$ is stable in probability.*

Concerning the convergence of ρ_t^z, we have the following theorem which is a stochastic version of the LaSalle invariance theorem. ρ_t^z is said to be Feller continuous if for fixed t, $E[G(\rho_t^z)]$ is continuous in z for any bounded continuous function G.

Theorem 5.3.3 (LaSalle invariance theorem) *Let $\mathscr{A}_\epsilon V \leq 0$ in Q_ϵ. Suppose Q_ϵ has compact closure, $\tilde{\rho}_t^z$ is Feller continuous, and that $Pr(||\tilde{\rho}_t^z - z|| > \delta) \to 0$ as $t \to 0$ for any $\delta > 0$, uniformly for $z \in Q_\epsilon$. Then ρ_t^z converges in probability to the largest invariant set contained in $C_\epsilon = \{x \in Q_\epsilon : \mathscr{A}_\epsilon V(x) = 0\}$ for almost all paths which never leave Q_ϵ.*

Let us first review some of the recent results for this stochastic stability problem. In [47], Mirrahimi & van Handel proposed a switching control for quantum spin systems to globally stabilize the angular moments at any eigenstate. The switching control operates a control input around a target state, which attracts the quantum states to the targets, and switches to another constant control input when the quantum states are near the other equilibrium points of the former control input in order to draw away from them. Their result can be state as

Theorem 5.3.4 *Consider the system* (5.30) *evolving in the set* S*. Let* $\rho_f = \rho_{\Psi_i}$ *and* $\gamma > 0$*. Consider the following control law:*

1. $u_t = -Tr(i[F_y, \rho_t]\rho_f)$ *if* $Tr(\rho_t \rho_f) \geq \gamma$*;*
2. $u_t = 1$ *if* $Tr(\rho_t \rho_f) \leq \gamma/2$*;*
3. *If* $\rho_t \in \mathcal{B} = \{\rho : \gamma/2 < Tr(\rho\rho_f) < \gamma\}$*, then* $u_t = -Tr(i[F_y, \rho_t]\rho_f)$ *if* ρ_t *last entered* $\mathcal{B}$ *through the boundary* $Tr(\rho\rho_f) = \gamma$*, and* $u_t = 1$ *otherwise.*

Then $\exists\, \gamma > 0$ *such that* u_t *globally stabilizes* (5.30) *around* ρ_f *and* $E\rho_t \to \rho_f$ *as* $t \to \infty$*.*

The proof is based on strict analysis on the sample paths of solutions. However, the ambiguity of finding the switching position γ prohibits the practical implementation of above control law. It will be more desirable to design a continuous control input to achieve the stochastic stability. The first work to try this is in [70]. Tsumura proposed a control law which globally stabilize the quantum spin system to the first eigenstate $\rho_f = \rho_{\psi_1}$ by continuous feedback.

Theorem 5.3.5 *Let* $\rho_f = \rho_{\psi_1}$*, then*

$$u_t = -\alpha Tr(i[F_y, \rho_t]\rho_f) + \beta V^I_{\rho_f}(\rho_t) \qquad \alpha, \beta > 0 \tag{5.38}$$

globally stabilizes system (5.30) *around* ρ_f *and* $E\rho_t \to \rho_f$ *as* $t \to \infty$ *when*

$$\frac{\beta^2}{8\alpha\eta} < 1 \tag{5.39}$$

Unfortunately, The continuous feedback law proposed by Tsumura can only globally stabilize the systems to the first eigenstate $\rho_f = \rho_{\Psi_1}$ or the last eigenstate $\rho_f = \rho_{\Psi_N}$.

We have performed a lot of numerical simulation to test the continuous feedback control law proposed by Tsumura. It turns out, the same approach can be applied to any performance functional $V_{\rho_f}(\rho)$ which satisfies $0 \leq V_{\rho_f}(\rho) \leq 1$ and $V_{\rho_f}(\rho) = 0$ if and only if $\rho = \rho_f$. The control functional $V_{\rho_f}^{III}$ in (5.36) is a good choice for low dimension spin systems.

Hence the contribution of our work is that, we find a feedback law u_t which is capable of global stabilizing the system (5.30) around any eigenstate as Mirrahimi and Handel did. In our feedback law, we do not require a sufficient condition like (5.39).

Our main Result can be stated as follows:

Claim: **[Main result]** *Consider the quantum spin system* (5.30) *evolving in the set* S. *Let* $\rho_f = \rho_{\psi_m}$, $m = 1, \ldots, N$, *we construct the control law*

$$u_1(\rho_t) = -Tr(i[F_y, \rho_t]\rho_f) \tag{5.40}$$

$$u_t = \alpha u_1 + \beta sign(u_1) V_{\rho_f}(\rho_t) \qquad \alpha, \beta > 0 \tag{5.41}$$

globally stabilizes system around ρ_f *and* $E\rho_t \to \rho_f$ *as* $t \to \infty$. *Here the sign function is defined as*

$$sign(x) = \begin{cases} 1 & x \geq 0 \\ -1 & x < 0 \end{cases}$$

the Lyapunov function $V_{\rho_f}(\rho_t)$ *has the properties:* $0 \leq V_{\rho_f}(\rho) \leq 1$ *and* $V_{\rho_f}(\rho) = 0$ *if and only if* $\rho = \rho_f$.

Remark: Note that $u_1(\rho_t)$ is the standard feedback control. By applying $u_1(\rho_t)$ alone, the convergence of ρ_t to an eigenstate is still random. This means, even the control u_1 becomes nearly 0 (inactive), the state ρ_t can converge to other undesired state. In our feedback law (5.40)-(5.41), we take the sign function with property, when $u_1 = 0$, $sign(u_1) = 1$. Hence if $\lim_{t\to\infty} \rho_t \neq \rho_f$ but on other eigenstates, then even though $u_1 = 0$, the control u_t is still active, because the value of Lyapunov function $V_{\rho_f}(\rho_t) = 1$, for instance for $V_{\rho_f}^I(\rho_t)$. In other words, the mechanism of the switching term in u_t is to draw the state ρ_t away from other undesired state.

Here we give some analysis we have so far for the proof of above claim. And more rigorous proof will be conducted in the future work. Numerical evidence of the above result will be shown in Section 5.4.

For the Lyapunov function $V_{\rho_f}(\rho_t)$, we take $V^I_{\rho_f}(\rho_t) = 1 - Tr(\rho_t\rho_f)$. Recall that in (5.41)

$$V^{II}_f(\rho_t) = 1 - Tr(\rho_t\rho_f)^2$$

by direct calculation, we obtain the generator

$$\begin{aligned}\mathcal{A}V^{II}_f =& -2Tr(\rho_t\rho_f)u_t u_1 - 4\eta(\lambda_f - Tr(F_z\rho_t))^2 Tr(\rho_t\rho_f)^2 \\ =& -2Tr(\rho_t\rho_f)(\alpha u_1^2 + \beta|u_1|V^I_{\rho_f}(\rho_t)) - X \leq 0\end{aligned}$$

Define the set $Q = \{\rho_t : V^{II}_f(\rho_t) < 1\}$. For $\rho_0 \in Q$, that is $V^{II}_f(\rho_0) < 1$, by Dynkin's Lemma, we have

$$E[V^{II}_f(\rho_t)] \leq V^{II}_{\tilde{f}}(\rho_0) - E[\int_0^t (Tr(\rho_t\rho_{\tilde{f}})(\alpha u_1^2 + \beta|u_1|V^I_{\rho_f}(\rho_t)) + X)ds]$$

since $E[V^{II}_{\tilde{f}}(\rho_t)]$ and $V^{II}_{\tilde{f}}(\rho_0)$ are bounded, so

$$E[\int_0^t (Tr(\rho_t\rho_f)(\alpha u_1^2 + \beta|u_1|V^I_{\rho_f}(\rho_t)) + X)ds] < \infty$$

By Borel-Cantelli Lemma,

$$Tr(\rho_t\rho_f)(\alpha u_1^2 + \beta|u_1|V^I_{\rho_f}(\rho_t)) + X \to 0 \quad \text{w.p.1}$$

By Lasalle Invariant Theorem, ρ_t converges in probability to the largest invariant set contained in the set $\{\mathcal{A}V^{II}_f = 0\} \cap Q = K$. In order to have the condition $\{\mathcal{A}V^{II}_f = 0\}$, we must have

$$\text{both} \quad u_1 = 0 \quad \text{and} \quad X = 0$$

since $X \geq 0$, and $X = 0$ only if $\rho_t = \rho_{\Psi_i} = \Psi_i\Psi_i^*$ for some $i = 1, \cdots, N$. It is also obvious that when $\rho_t = \rho_{\Psi_i}$, we have $u_1 = 0$. Thus the only probabilities are $V^{II}_{\rho_f}(\rho_t) = 0$ for $\rho_t = \rho_f$ or $V^{II}_{\rho_f}(\rho_t) = 1$ for $\rho_t = \rho_{\Psi_i}$, $i \neq f$. To remain in the set K, so $\rho_t \to \rho_f$ and ρ_f is stable in probability.

Next we are going to show if ρ_0 lies in the set $S_1 = \{\rho : V^{II}_f(\rho) = 1\}$, for almost all paths ρ_t will exit the set S_1 in finite time by the feedback law. On S_1, we have $u_1 = 0$, set $\beta = 1$, then $u_t = 1$. We utilize the following Lemma which is proved in [47].

Lemma 5.3.1 *For a fixed time $T > 0$, define the nonnegative function*

$$\chi(\rho_t) = \min_{t\in[0,T]} \mathbb{E}V^I(\rho_t)$$

with the control $u_t = 1$,then $\chi(\rho_t) < 1$, $\forall\, \rho \in S_1$. Here $\mathbb{E}V$ denotes the expectation of V.

By Lemma 5.3.1, we see ρ_t will exit the set S_1 in finite time by the feedback law.

5.4 Numerical Method and Numerical Results

In [47], it is showed that the set of nonnegative nonzero matrices ρ_t is almost sure invariant for the system (5.30).

$$d\rho_t = -iu_t[F_y, \rho_t]dt - \frac{1}{2}[F_z, [F_z, \rho_t]]dt + \sqrt{\eta}(F_z\rho_t + \rho_t F_z - 2Tr(F_z\rho_t)\rho_t)dW_t$$

Hence it is essential to develop a numerical method to preserve the nonnegative definiteness properties of the density matrix. Our discretization for the system is based on the operator splitting technique and the implicit Euler method. We show the proposed scheme is a nonnegativity-preserving scheme.

The most well-known numerical method for solving ODE is given by the Euler method. Consider the stochastic differential equation in the form of

$$dX_t = a(t, X_t)dt + b(t, X_t)dW_t \tag{5.42}$$

where $a, b : [0, T] \times \mathbb{R} \to \mathbb{R}$ are the drift and diffusion parts, and $W_t : 0 \leq t \leq T$ the Wiener process. The scheme of the explicit Euler method is given by

$$X_{n+1} = X_n + a(t_n, X_n)\Delta_n + b(t_n, X_n)\Delta W_n \tag{5.43}$$

Some drawback of the explicit Euler method are being lack of numerical stability and some problems with the geometrical invariance properties. To overcome these drawbacks, we use the so called drift-implicit Euler method in the form of

$$X_{n+1} = X_n + a(t_{n+1}, X_{n+1})\Delta_n + b(t_n, X_n)\Delta W_n \tag{5.44}$$

For the system (5.30), we apply operator splitting technique on the deterministic and stochastic term, then apply the implicit Euler method on the drift term

$$\hat{\rho} = \sqrt{\eta}(F_z\rho_n + \rho_n F_z - 2Tr(F_z\rho_n)\rho_n)dW_t \tag{5.45}$$

$$\frac{\rho_{n+1} - \hat{\rho}}{\Delta t} = -iu_t[F_y, \rho_{n+1}] - \frac{1}{2}[F_z, [F_z, \rho_{n+1}]] \tag{5.46}$$

Equation (5.46) can be equivalently written as

$$A\rho_{n+1} + \rho_{n+1}A^T = \hat{\rho} + F_z\rho_{n+1}F_z\Delta t \tag{5.47}$$

where $A = \frac{I}{2} + u\Delta t F_y + \frac{\Delta t}{2} F_z^2$, which is a skew-symmetric matrix.

To show that the scheme defined by (5.45) (5.46) is nonnegative definite preserving for ρ_t, we utilize the following two propositions.

Proposition 5.4.1 *For given $\hat{\rho}$, there is a unique solution ρ_{n+1} for the equation* (5.47)*.*

Proof: We consider the iteration

$$A\rho^{k+1} + \rho^{k+1}A^T = \hat{\rho} + F_z\rho^k F_z\Delta t \tag{5.48}$$

which is initialized by $\rho^0 = \hat{\rho}$. To show that this iteration defines a contraction mapping, we define

$$A\rho^* + \rho^* A^T = \hat{\rho} + F_z\rho^* F_z\Delta t$$

Subtract the above two equations,

$$A(\rho^{k+1} - \rho^*) + (\rho^{k+1} - \rho^*)A^T = F_z(\rho^k - \rho^*)A^T$$

multiply both sides by $(\rho^{k+1} - \rho^*)$, we get

$$\|\rho^{k+1} - \rho^*\|^2 + \|F_z(\rho^{k+1} - \rho^*)\|^2\Delta t = (\rho^{k+1} - \rho^*)F_z(\rho^k - \rho^*)F_z\Delta t \tag{5.49}$$

where $\|\cdot\|$ defines the matrix Frobenius norm. We get the estimation

$$\|\rho^{k+1} - \rho^*\|^2 < \|F_z\|^2\|\rho^{k+1} - \rho^*\|\|\rho^k - \rho^*\|\Delta t$$

$$\|\rho^{k+1} - \rho^*\| < M\Delta t\|\rho^k - \rho^*\|$$

where $M = \|F_z\|^2 = \frac{J(J+1)(2J+1)}{3}$. Choosing Δt such that $\gamma = M\Delta t < 1$ we obtain a contraction map, so $\rho^k \to \rho^*$ as $k \to \infty$.

Proposition 5.4.2 *For the equation $A\rho + \rho A^T = \tilde{\rho}$, assuming the operator e^{As} is exponentially stable, then it has the solution of form*

$$\rho = \int_0^\infty e^{As}\tilde{\rho}e^{A^T s}ds \tag{5.50}$$

Hence if $\tilde{\rho}$ is a nonnegative definite matrix, so is ρ.

Proof: Suppose ρ is given in the form of (5.50). Let $s = t - \sigma$, then

$$\rho = \int_{-\infty}^{t} e^{A(t-\sigma)} \tilde{\rho} e^{A^T(t-\sigma)} d\sigma$$

since ρ is independent of σ,

$$0 = \frac{d\rho}{d\sigma} = A\rho + \rho A^T + \tilde{\rho}$$

if $\tilde{\rho}$ is a nonnegative definite matrix, for any vector e^{As}, $e^{As}\tilde{\rho}e^{A^T s} \geq 0$. so ρ is also a nonnegative definite matrix.

As ρ_t is a $N \times N$ complex matrix, the SDE for ρ_t is equivalent to a N^2 number of SDEs for each entry of ρ_t. We first reshape the density matrix ρ to be an N^2 dimensional vector whose elements are taken column-wise from ρ. The equation (5.45) can be rewritten as

$$\hat{\rho} = C\rho_n dW_t \tag{5.51}$$

for some $N^2 \times N^2$ matrix C, then

$$\hat{\rho} = e^{(CW_n - \frac{1}{2}C^2\Delta t))}\rho_n;$$

Which gives a nonnegative definite density matrix $\hat{\rho}$ provided that ρ_n is nonnegative definite. In summary, the scheme (5.45) (5.46) gives a nonnegativity-preserving scheme.

Next, we demonstrate the efficiency of the proposed feedback law (5.40)-(5.41) by using numerical simulation. We consider the spin system where $J = 2$, corresponding to low dimensional case ($N = 5$), and $J = 5$ for high dimension ($N = 11$). The initial state ρ_0 is a randomly generated Hermitian matrix. The target state ρ_f is set to be

$$\rho_f = \rho_{\Psi_k} \quad \text{where} \quad k = J + 1$$

as this equilibrium state is the most difficult one to be stabilized.

In the feedback control, we set $\alpha = 1$, $\beta = 1$, and choose $V_{\rho_f}(\rho_t)$ to be $V^I_{\rho_f}(\rho_t)$ in (5.36). By using Monte Carlo simulation, we plot the figures showing the relationship between time T and performance V. Figure 5.2 shows a typical trajectory for case when $J = 2$ and $J = 5$ with detector efficiency $\eta = 0.1$. It is observed the performance V goes to 0 as time T increases, which results $\rho_t \to \rho_f$. And when the dimension of the spin system increases, it takes longer time to stabilize to the target equilibrium.

As shown before for the deterministic case $\eta = 0$, the quantum state will not converge to any equilibrium states ρ_f. Hence the detector efficiency η is essential for this stabilization problem. With large η, the stabilization of the quantum spin system can be achieved in short time. Especially for high dimensional spin system, it requires large detector efficiency η. Figure 5.3 demonstrates this result. Here $\eta = 0.01$ comparing to $\eta = 0.1$ previously, we observe that it takes around $T = 700$ to stabilize the spin system of $J = 5$.

As long as the feedback law works, β can be kept large in order to have large control magnitude.

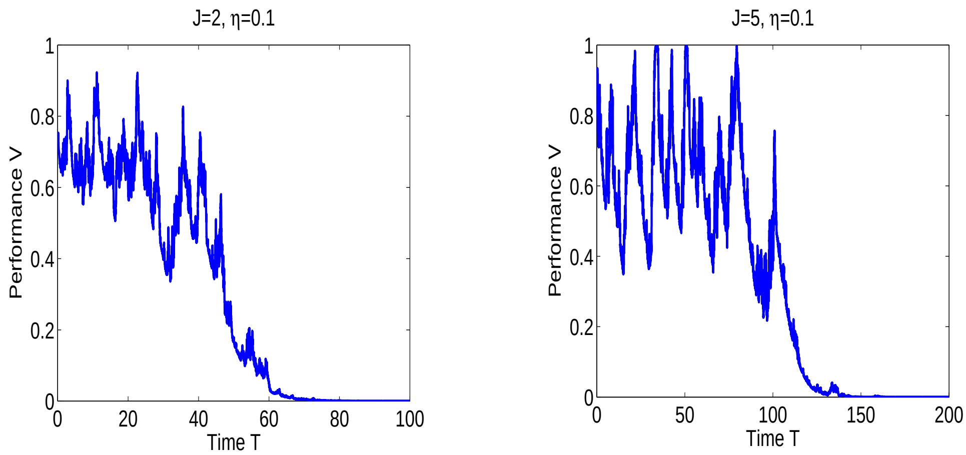

Figure 5.2: Transition of performance $V^I_{\rho_f}(\rho_t)$ for the quantum spin system with $J = 2$, $J = 5$ and $\eta = 0.1$

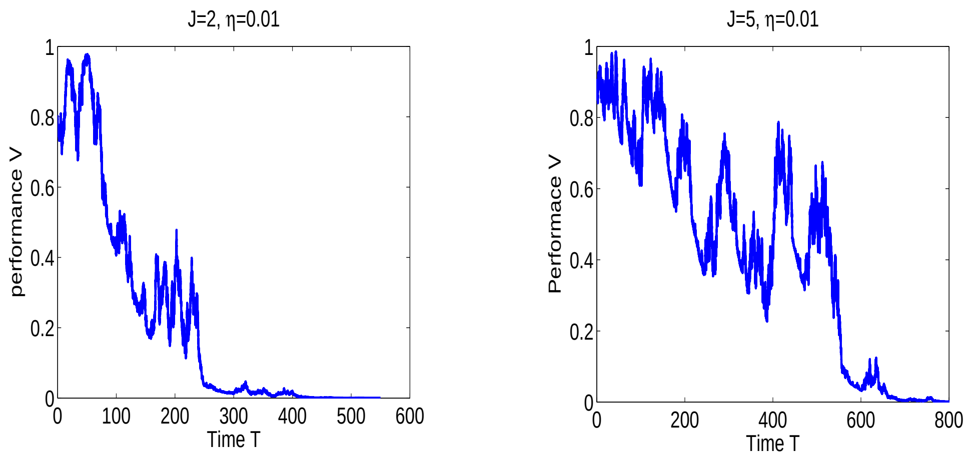

Figure 5.3: Transition of performance $V^I_{\rho_f}(\rho_t)$ for the quantum spin system with $J = 2$, $J = 5$ and $\eta = 0.01$

Chapter 6

Time Optimal Control on Linear and Bilinear Systems

In this chapter, we propose a numerical method, based on semi-smooth Newton method, to solve time optimal control problem with discontinuous (bang-bang) control. A regularized problem is formulated and the asymptotic and monotone behavior of the regularization procedure is investigated. For the regularized problem, semi-smooth Newton method is applied to solve the optimality system. Several numerical tests are presented which demonstrate the capability of our proposed approach.

6.1 Introduction

We consider the following optimal control problem with a scalar state constraint and a scalar control

$$\min \int_0^T g(u(t), x(t))dt + h(x(T)) \tag{6.1}$$

$$\text{subject to} \quad \frac{dx(t)}{dt} = f(u(t), x(t)), \quad t \in [0, T]; \tag{6.2}$$

$$x(0) = x_0; \quad \Phi(x(T)) = 0 \tag{6.3}$$

where the state variable $x(t) \in \mathbb{R}^n$, the admissible control $u(t) \in \mathcal{U}$,

$$\mathcal{U} = \{u(t) \in \mathbb{R} \text{ is measureable}\}$$

the running cost functional $g : \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}$, terminal cost functional $h : \mathbb{R}^n \to \mathbb{R}$, dynamics $f \in \mathbb{R} \times \mathbb{R}^n \to \mathbb{R}^n$ and state constraint $\Phi : \mathbb{R}^n \to \mathbb{R}$. We assume that functions f, g, h are differentiable functions.

In the thesis, we will study three types of control problem in the general form of (6.1)-(6.3), which we denote as problem $(\mathcal{P})$. They are minimum norm problem, time optimal control problem, minimum effort control problem.

Minimum norm problem:

For a fixed time horizon T, there is not constraint in the admissible control, and the cost functional to be minimized is in the form of

$$\min \quad \int_0^T \frac{|u(t)|^2}{2}\, dt$$

that is, the running cost functional $g = \frac{|u(t)|^2}{2}$ and the terminal cost functional $h = 0$.

Time optimal control problem:

We assume the admissible control $u(t)$ is constrained, for example,

$$|u(t)| \leq \gamma$$

for some scalar $\gamma > 0$. Instead of having a fixed time horizon T, the time optimal control problem is to find the least time T to drive the state variable $x(t)$ from x_0 to the target satisfying $\Phi(x(T)) = 0$. The cost functional to be minimized is in the form of

$$\min \quad T = \int_0^T 1\, dt$$

that is, the running cost functional $g = 1$ and the terminal cost functional $h = 0$.

Minimum effort control problem:

Minimum effort control problem is to answer the following question: How small the control effort can be made in order to drive the system to a target within fixed time T? This is a counterpart for the time optimal control problem. We define the effort to be the maximum norm of $u(t)$, $\|u\| = sup_{0 \leq t \leq T} |u(t)|$. Since the control $|u(t)| \leq \gamma$, the cost functional to be minimized is

$$\min \quad \gamma$$

6.2 The Time Optimal Control Problem and Its Regularization

Standard technique to solve the control problem $(\mathcal{P})$ is to form the necessary optimality system by using Pontryagin's maximum principle first, then solve the derived two-point boundary value problem using iterative methods.

We introduce the costate $p(t) \in \mathbb{R}^n$, and define the Hamiltonian

$$H(x(t), u(t), p(t), t) = g(u(t), x(t)) + p^T(t)[f(u(t), x(t)] \tag{6.4}$$

Let $(x^*(t), p^*(t), u^*(t))$ be the optimal pair for problem $(\mathcal{P})$, the first order necessary optimality conditions are given by Pontryagin's maximum principle

$$\frac{dx^*(t)}{dt} = \frac{\partial H}{\partial p}(x^*(t), u^*(t), p^*(t), t), \quad x(0) = x_0 \tag{6.5}$$

$$-\frac{dp^*(t)}{dt} = \frac{\partial H}{\partial x}(x^*(t), u^*(t), p^*(t), t) \tag{6.6}$$

$$u^*(t) = \text{argmin}_{u \in \mathcal{U}} H(x^*(t), u(t), p^*(t), t) \tag{6.7}$$

with transversality conditions,

$$\Phi(x^*(T)) = 0 \tag{6.8}$$

$$p^*(T) = \frac{\partial \Psi}{\partial x}(x(t), u(t), p(t), t)|_{t=T} \tag{6.9}$$

with

$$\Psi(x(t), u(t), p(t), t) = h(x(t)) + \mu\Phi(x(t))$$

where μ is another scalar valued Lagrange multiplier for the boundary condition (6.3). If the $x(T)$ is specified, i.e. $x(T) = x_f$ for some prescribed value x_f, then $\mu = 0$.

For the time optimal control problem where the final time T is a free variable, there is additional transversality condition. That is, the Hamiltonian must be identically zero when evaluate on an optimal trajectory

$$H(x^*(t), u^*(t), p^*(t), t) = 0 \quad \text{for } t \in [0, T] \tag{6.10}$$

Hence solving the original optimal control problem $(\mathcal{P})$ can be equivalent to solve the optimality system (6.5)-(6.10), which is a two point boundary value problem.

For time optimal control problem, the associated optimality system is complicated due to nonsmoothness of the optimal controls. In fact, the first order optimality system for time optimal control problems contains a switching operation which impedes the use of fast numerical methods. Hence our approach is first to introduce a regularization to the time optimal problem. We will show the solution of the regularized problem will converge to the solution of time optimal control problem asymptotically. For simplicity, we describe the regularization process for time optimal control problem for the linear system. The same process can be applied to bilinear system also.

Consider the time-optimal control problem for the linear multi-input system with prescribed fixed boundary points and constrained control.

$$\begin{cases} \min\limits_{\tau \geq 0} \displaystyle\int_0^\tau dt \\ \text{subject to} \qquad \dfrac{d}{dt}x(t) = Ax(t) + Bu(t),\ \ x(0) = x_0,\ x(\tau) = x_f, \\ |u(t)|_{\ell^\infty} \leq 1 \end{cases} \tag{P}$$

where $A \in \mathbb{R}^{n \times n}$, $B \in \mathbb{R}^{n \times m}$, $x_0 \in \mathbb{R}^n$, $x_1 \in \mathbb{R}^n$ are given, the control $u(t) \in \mathbb{R}^m$ is measurable, and $|\cdot|_{\ell^\infty}$ denotes the infinity-norm on $\mathbb{R}^m$. It is assumed that the system is controllable, that is, x_1 can be reached in finite time by an admissible control. Then (P) admits a solution with optimal time denoted by τ^*, and associated state x^* and control u^*.

The first order optimality system for (P) can be expressed in terms of the costate $p(t)$ and the Hamiltonian

$$H(x, u, p) = 1 + p^T(Ax + Bu),$$

as

$$\begin{cases} \dot{x} = Ax + Bu,\ x(0) = x_0,\ x(\tau) = x_f, \\ -\dot{p} = A^T p, \\ u = argmin_{|u|_{\ell^\infty} \leq 1} H(x, u, p), \\ 1 + p(t)^T(Ax(t) + Bu(t)) = 0,\ \forall\, t \in [0, \tau], \end{cases} \tag{6.11}$$

Throughout the chapter, we use the notation $\dot{x}$ to denote $\frac{dx(t)}{dt}$. To minimize the Hamiltonian subject to be the control constraint, we find that

$$u(t) = -\text{sign}(B^T p(t))$$

where the sign function is defined as

$$\operatorname{sign}(x) = \begin{cases} [-1, 1] & x = 0 \\ \dfrac{x}{|x|} & |x| > 0, \end{cases}$$

We see the control $u(t)$ is in bang-bang natural, which prohibits the use of Newton-type methods to solve for solving the optimality system (6.11) numerically. Therefore, we consider a family of regularized problem

$$\begin{cases} \min_{\tau \geq 0} \displaystyle\int_0^\tau (1 + \frac{\varepsilon}{2}\, |u(s)|^2)\, ds \\ \text{subject to} \qquad \dfrac{d}{dt} x(t) = Ax(t) + Bu(t),\ \ x(0) = x_0,\, x(\tau) = x_f, \\ |u(t)|_{\ell^\infty} \leq 1. \end{cases} \tag{P_ε}$$

with $\varepsilon > 0$. The norm $|\cdot|$ used in the cost-functional denotes the Euclidean norm.

We see the regularized problem adds the $\frac{\varepsilon}{2}\, |u(s)|^2$ term in the cost functional to be minimized. As $\varepsilon \to 0$, the cost functional in (P_ε) converges to the original cost functional in (P). To be more precise, we argue the convergence of the solutions $(x_\varepsilon,\, p_\varepsilon, u_\varepsilon, \tau_\varepsilon)$ of (P_ε) to a solution $(x^*,\, p^*,\, u^*,\, \tau^*)$ of (P) next. Here we utilize the results stated in [32].

Proposition 6.2.1 *For every $0 < \varepsilon_0 < \varepsilon_1$ and any solution $(\tau^*,\, u^*)$ of (P) we have*

$$\tau^* \leq \tau_{\varepsilon_0} \leq \tau_{\varepsilon_1} \leq \tau^*(1 + \frac{\varepsilon_1}{2}), \tag{6.12}$$

$$|u_{\varepsilon_1}|_{L^2(0,\, \tau_{\varepsilon_1})} \leq |u_{\varepsilon_0}|_{L^2(0,\, \tau_{\varepsilon_0})} \leq |u^*|_{L^2(0,\, \tau^*)}. \tag{6.13}$$

Proof: From the definition of τ^* and τ_ε we have

$$\tau^* \leq \tau_\varepsilon \quad \text{for every} \ \ \varepsilon > 0,$$

and

$$\tau_\varepsilon + \frac{\varepsilon}{2} \int_0^{\tau_\varepsilon} |u_\varepsilon|^2 \leq \tau^* + \frac{\varepsilon}{2} \int_0^{\tau^*} |u^*|^2,$$

hence

$$|u_\varepsilon|_{L^2(0,\, \tau_\varepsilon)} \leq |u^*|_{L^2(0,\, \tau^*)}$$

since $|u^*|_{\ell^\infty} \leq 1$, then

$$\tau^* \leq \tau_\varepsilon \leq \tau^*(1 + \frac{\varepsilon}{2})$$

For $0 < \varepsilon_0 < \varepsilon_1$, by the minimum property of τ_{ε_0}, we have

$$\int_0^{\tau_{\varepsilon_0}} (1 + \frac{\varepsilon_0}{2}\,|u_{\varepsilon_0}|^2) \leq \int_0^{\tau_{\varepsilon_1}} (1 + \frac{\varepsilon_1}{2}\,|u_{\varepsilon_1}|^2).$$

By adding $\frac{1}{2}(\varepsilon_1 - \varepsilon_0)\int_0^{\tau_{\varepsilon_1}}\,|u_{\varepsilon_1}|^2$ on both sides, we have the following inequalities

$$\tau_{\varepsilon_0} + \frac{\varepsilon_1}{2}\int_0^{\tau_{\varepsilon_1}}\,|u_{\varepsilon_1}|^2 + \frac{\varepsilon_0}{2}\big(\int_0^{\tau_{\varepsilon_0}}\,|u_{\varepsilon_0}|^2 - \int_0^{\tau_{\varepsilon_1}}\,|u_{\varepsilon_1}|^2\big)$$

$$\leq \int_0^{\tau_{\varepsilon_1}}\,(1 + \frac{\varepsilon_1}{2}\,|u_{\varepsilon_1}|^2) \leq \tau_{\varepsilon_0} + \frac{\varepsilon_1}{2}\int_0^{\tau_{\varepsilon_0}}\,|u_{\varepsilon_0}|^2. \quad (6.14)$$

Estimating the first with the last expression in (6.14) implies that

$$\varepsilon_1\big(\int_0^{\tau_{\varepsilon_1}}\,|u_{\varepsilon_1}|^2 - \int_0^{\tau_{\varepsilon_0}}\,|u_{\varepsilon_0}|^2\big) \leq \varepsilon_0\big(\int_0^{\tau_{\varepsilon_1}}\,|u_{\varepsilon_1}|^2 - \int_0^{\tau_{\varepsilon_0}}\,|u_{\varepsilon_0}|^2\big),$$

and since $\varepsilon_0 < \varepsilon_1$ hence

$$|u_{\varepsilon_1}|_{L^2(0,\,\tau_{\varepsilon_1})} \leq |u_{\varepsilon_0}|_{L^2(0,\,\tau_{\varepsilon_0})}. \quad (6.15)$$

Estimating the first with the second expression in (6.14) we obtain

$$\tau_{\varepsilon_0} + \frac{\varepsilon_0}{2}\,|u_{\varepsilon_0}|^2_{L^2(0,\,\tau_{\varepsilon_0})} \leq \tau_{\varepsilon_1} + \frac{\varepsilon_0}{2}\,|u_{\varepsilon_1}|^2_{L^2(0,\,\tau_{\varepsilon_1})}$$

and by (6.15), we obtain

$$\tau^* \leq \tau_{\varepsilon_0} \leq \tau_{\varepsilon_1}.$$

The Proposition (6.2.1) implies the monotonicity of solution (u, τ) with respect to the parameter ε. From (6.12), we see τ_ε is bounded below and above by τ^*. Let $\varepsilon \to 0$, we have $\tau_\varepsilon \to \tau^*$. The following theorem gives the asymptotic properties of solutions of regularized problems.

Theorem 6.2.1 *For $\varepsilon \to 0^+$ we have $\tau_\varepsilon \to \tau^*$ and every convergent subsequence of solutions $\{(u_\varepsilon,\, x_\varepsilon)\}_{\varepsilon>0}$ of (P_ε) converges in $L^2(0,\, \tau_\epsilon; \mathbb{R}^m) \times W^{1,2}(0,\, \tau_\epsilon;\, \mathbb{R}^n)$ to a solution $(u^*,\, x^*)$ of* (P).

Here the convergence of u_ε to u^* is defined as

$$\int_0^1\,|u_\varepsilon(\tau_\varepsilon\, t) - u^*(\tau^*\, t)|^2\, dt \to 0$$

and analogously for $\{x_\varepsilon\}$, and for weak convergence.

Proof: By Proposition 6.11, $\tau_\varepsilon \to \tau^*$ follows. Since $\{u_\varepsilon(\tau_\varepsilon\cdot)\}_{\varepsilon>0}$ and $\{x_\varepsilon(\tau_\varepsilon\cdot)\}_{\varepsilon>0}$ are bounded sequences in $L^2(0,\,1;\mathbb{R}^m)$ and $W^{1,2}(0,\,1;\,\mathbb{R}^n)$, by Alaoglu's theorem, there exist weak accumulation points $u^* \in L^2(0,\tau^*;\mathbb{R}^m)$, and $x^* \in W^{1,2}(0,\,\tau^*;\,\mathbb{R}^n)$. Here we avoid subsequential indices. By passing the limit in $\dot{x}_\varepsilon(\tau_\varepsilon\,\cdot) = \tau_\varepsilon(Ax_\varepsilon(\tau_\varepsilon\,\cdot)+Bu_\varepsilon(\tau_\varepsilon\,\cdot))$ and $x_\varepsilon(0) = x_0,\ x_\varepsilon(\tau_\varepsilon) = x_1$ it follows that x^* is admissible. Due to weak closure of $\{u \in L^2(0,\,1;\mathbb{R}^m) : |u(x)|_{\ell^\infty} \le 1\, a.e.\}$ we have that u^* is admissible as well. Since

$$\lim_{\varepsilon\to 0^+} \tau_\varepsilon + \frac{\varepsilon}{2}\int_0^{\tau_\varepsilon} |u_\varepsilon|^2 = \tau^*,$$

the triple $(\tau^*,\,u^*,\,x^*)$ is optimal for problem (P). By Proposition 6.2.1 and weak lower semi-continuity of norms

$$\limsup_{\varepsilon\to 0}\ |u_\varepsilon|_{L^2(0,\tau_\varepsilon)} \le |u^*|_{L^2(0,\tau^*)} \le \liminf_{\varepsilon\to 0}\ |u_\varepsilon|_{L^2(0,\tau_\varepsilon)} \tag{6.16}$$

and hence $\lim_{\varepsilon\to 0} |u_\varepsilon|_{L^2(0,\tau_\varepsilon;\mathbb{R}^m)} = |u^*|_{L^2(0,\tau^*;\mathbb{R}^m)}$. As a consequence u_ε and x_ε converges strongly in $L^2(0,\,\tau_\varepsilon)$, respectively $W^{1,2}(0,\,\tau_\varepsilon;\,\mathbb{R}^n)$, to u^* and x^*.

To show the uniqueness of the optimal solution for (P), Let $\hat{u}$ denote another optimal control for (P) with $|\hat{u}| < |u^*|$. Then by (6.13) and (6.16)

$$\limsup_{\varepsilon\to 0}\ |u_\varepsilon|_{L^2(0,\tau_\varepsilon;\mathbb{R}^m)} \le |\hat{u}|_{L^2(0,\tau^*;\mathbb{R}^m)} < |u^*|_{L^2(0,\tau^*;\mathbb{R}^m)} \le \liminf_{\varepsilon\to 0}\ |u_\varepsilon|_{L^2(0,\tau_\varepsilon;\mathbb{R}^m)},$$

which is a contradiction. Consequently (P) has a minimal norm control and the claimed strong convergence properties hold.

Theorem 6.2.1 gives the wellposeness of the regularization of the original time optimal control problem. It states that by solving the regularized problem with small $\varepsilon > 0$, we are able to get the solution to the time optimal control problem asymptotically. Now let us turn to the optimality condition for (P_ε).

Define the Hamiltonian

$$H = 1 + \frac{\varepsilon}{2}|u|^2 + p^T(Ax + uB)$$

By Pontryagin's maximum principle, to minimize the Hamiltonian over all the admissible control, it is equivalent to have $\frac{\partial H}{\partial u} = 0$,

$$\varepsilon u + B^T p = 0$$

hence

$$u = \begin{cases} -1 & \text{if } B^T p > \varepsilon \\ -\frac{B^T p}{\varepsilon} & \text{if } |B^T p| \leq \varepsilon \\ 1 & \text{if } B^T p < -\varepsilon. \end{cases} \tag{6.17}$$

We define

$$\text{sign}_\varepsilon(x) = \begin{cases} -1 & \text{if } x \leq -\varepsilon \\ \frac{x}{\varepsilon} & \text{if } |x| < \varepsilon \\ 1 & \text{if } x \geq \varepsilon. \end{cases} \tag{6.18}$$

then the control u in (6.17) can be written as $u = -\text{sign}_\varepsilon(B^T p)$. Note that $\text{sign}_\varepsilon(x)$ is also known as the Yosida approximation for the sign function $\text{sign}(x)$.

The necessary optimality system for (P_ε) is

$$\begin{cases} \dot{x} = Ax + Bu_\varepsilon,\ x(0) = x_0,\ x(\tau_\varepsilon) = x_f \\ -\dot{p} = A^T p \\ u_\varepsilon = -\text{sign}_\varepsilon(B^T p) \\ 1 + \frac{\epsilon}{2}|u_\varepsilon(\tau_\varepsilon)|^2_{\mathbb{R}^m} + p(\tau_\varepsilon)^T(Ax(\tau_\varepsilon) + Bu_\varepsilon(\tau_\varepsilon)) = 0. \end{cases} \tag{6.19}$$

Since the time optimal τ is a free variable, it will be expensive to have time integrate on state and costate with varying time horizon τ. Hence we scale the time horizon from $[0, \tau]$ to $[0, 1]$ by change of variable. Let $\hat{t} = \frac{t}{\tau}$, and setting

$$\hat{x}(\hat{t}) = x(\tau\hat{t}) = x(t),\ \hat{p}(\hat{t}) = p(\tau\hat{t}) = p(t),\ \hat{u}(\hat{t}) = u(\tau\hat{t}) = u(t),$$

we obtain the following equivalent system to (6.19),

$$\begin{cases} \dot{x} = \tau(Ax + Bu),\ x(0) = x_0,\ x(1) = x_f \\ -\dot{p} = \tau A^T p \\ u = -\text{sign}_\varepsilon(B^T p) \\ 1 + \frac{\epsilon}{2}|u(1)|^2 + p(1)^T(Ax(1) + Bu(1)) = 0, \end{cases} \tag{6.20}$$

Here for convenience of notation the dependence on ε and the superscript $^\wedge$ were dropped.

To summarize, for the time optimal control problem, the control law is nonsmooth, which prohibits the usage of Newton-type method directly. To overcome this difficulty, we formulate a regularized problem (P_ε) with parameter $\varepsilon > 0$ for the time optimal control problem. The solution of the regularized problem converges asymptotically to the solution of the time optimal control problem as $\varepsilon \to 0^+$. To solve for the regularized problem, the necessary optimality system (6.20) is formulated, which is a two point boundary value problem.

6.3 Semi-smooth Newton Method

In this section, we describe the semi-smooth Newton method for solving the regularized optimality system (6.20). It will allow (6.20) to be solved efficiently in spite of the fact that $\mathrm{sign}_\varepsilon$ is not differentiable.

We introduce the function

$$F : D_F \subset X \to L^2(0,1;\mathbb{R}^n) \times L^2(0,1;\mathbb{R}^n) \times U \times \mathbb{R}^n \times \mathbb{R}$$

where

$$D_F = W^{1,2}(0,1) \times \mathcal{U}_{p_\varepsilon} \times U \times \mathbb{R},$$
$$X = W^{1,2}(0,1;\mathbb{R}^n) \times W^{1,2}(0,1;\mathbb{R}^n) \times U \times \mathbb{R},$$

and

$$F(x,\, p,\, u,\, \tau) = \begin{pmatrix} \dot{x} - \tau A x - \tau B u \\ -\dot{p} - \tau A^T p \\ u + \mathrm{sign}_\varepsilon(B^T p) \\ x(1) - x_f \\ 1 + \frac{\varepsilon}{2}|u(1)|^2 + p(1)^T\left(Ax(1) + Bu(1)\right) \end{pmatrix}. \tag{6.21}$$

Applying Newton's method to solve $F = 0$ is impeded by the non-differentiability of the function $\mathrm{sign}_\varepsilon$. Hence we use a generalized derivative

$$G_\varepsilon(x) := \begin{cases} \frac{1}{\varepsilon} & \text{if } |x| < \varepsilon \\ 0 & \text{if } |x| \geq \varepsilon \end{cases} \tag{6.22}$$

the resulting Newton iteration is semi-smooth and hence locally superlinearly convergent. Detailed proof can be found in [32]. The Newton iteration step is given by

$$DF(x,\, p,\, u,\, \tau)(\delta x,\, \delta p,\, \delta u,\, \delta\tau) = -F(x,\, p,\, u,\, \tau) \tag{6.23}$$

where $\delta x(0) = 0$ and DF is the Jacobian, which consists of the Frechet-derivative in all terms of F except for $p \to \mathrm{sign}_\varepsilon(B^T p)$, for which the generalized derivative is taken according to (6.22). We give the detailed form of (6.23):

$$\begin{cases} \frac{d}{dt}\delta x - \tau A\delta x - \tau B\,\delta u - \delta\tau(Ax + Bu) = -F_1, \quad \delta x(0) = 0 \\ -\frac{d}{dt}\delta p - \tau A^T\delta p - \delta\tau A^T p = -F_2 \\ \delta u + G_\varepsilon(B^T p)B^T\delta p = -F_3 \\ \delta x(1) = -F_4 \\ p(1)^T(A\delta x(1) + B\delta u(1)) + \delta p(1)^T(Ax(1) + Bu(1)) \\ \qquad\qquad\qquad\qquad\qquad + \varepsilon u(1)^T\delta u(1) = -F_5, \end{cases} \tag{6.24}$$

where $F = (F_1, \ldots, F_5)$ are given by (6.21).

With a good initial guess of $(x(t), p(t), u(t), \tau)$ for $t \in [0, 1]$ sufficiently close to the solution $(x_\varepsilon(t), p_\varepsilon(t), u_\varepsilon(t), \tau_\varepsilon)$, the semi-smooth Newton algorithm (6.24) converges superlinearly. It is obvious that the resulting Jacobian DF can be of high dimension with initialization for every $t \in [0, 1]$. Hence in order to solve the semi-smooth Newton algorithm (6.24) more efficiently, we compute a reduced Jacobian with some shooting parameters by integrating the state $x(t)$ and costate $p(t)$ and variation of them in the regularized optimality system (6.20) forwards and backwards.

For instance, let the shooting parameters be $z = (p(1), \tau) \in \mathbb{R}^{n+1}$. The first three component (F_1, F_2, F_3) in (6.21) can be solved as an initial value problem. The other two component (F_4, F_5) form the new shooting function Ψ.

The first three equations in the variational form (6.24) can be solved as a system, which is equivalent to

$$\frac{d}{dt}\begin{pmatrix} \delta x(t) \\ \delta p(t) \end{pmatrix} = \tau \begin{pmatrix} A & -G_\epsilon(B^T p)BB^T \\ 0 & A^T \end{pmatrix} \begin{pmatrix} \delta x(t) \\ \delta p(t) \end{pmatrix} + \begin{pmatrix} Ax(t) + u(t)B \\ A^T p(t) \end{pmatrix} \delta\tau + \begin{pmatrix} f \\ g \end{pmatrix} \tag{6.25}$$

Since $x(0)$ is fixed, i.e. $\delta x(0) = 0$. After solving the variational systems (6.25), we have

$$\delta x(1) = C\delta p(1) + D\delta\tau + E \tag{6.26}$$

for some $C, D \in \mathbb{R}^{n\times n}$ and $E \in \mathbb{R}^n$.

Substitute (6.26) into the last two equations of (6.24), the reduced form of the semi-smooth Newton iteration is given by

$$J \begin{pmatrix} \delta p(1) \\ \\ \delta\tau \end{pmatrix} = \begin{pmatrix} r_1 \\ \\ r_2 \end{pmatrix}. \tag{6.27}$$

The reduced Jacobian J is in $\mathbb{R}^{(n+1)\times(n+1)}$. Assuming it is invertible, then the update can be used for

$$\begin{aligned} p(1)^{(k+1)} &= p(1)^{(k)} + \alpha\delta p(1) \\ \tau^{(k+1)} &= \tau^{(k)} + \alpha\delta\tau \end{aligned}$$

where $\alpha \in (0, 1]$ is the damping factor, and k is the number of iteration.

The algorithm for solving the regularized optimality system (6.20) for linear system using semi-smooth Newton method can be described as follows:

1. Set $k = 0$ and select an initial guess of $p(1)^{(0)}$ and $\tau^{(0)}$;
2. Integrate the costate $p(t)$ backwards in time from $t = 1$ to 0, and compute $u(t)$ simultaneously;
3. Integrate the state $x(t)$ forwards in time from $t = 0$ to 1 and record terminal state $x(1)$;
4. Form the Jacobian for the semi-smooth Newton method where the generalized derivative of $\mathrm{sign}_\varepsilon$ is taken as G_ε, solve the system of equations (6.27) for the update $\delta z = (\delta p(1), \delta\tau)$;
5. Determine the damping factor $\alpha^{(k)} \in (0, 1]$ by line search method so as to minimize

   $$\min_{\alpha\in(0,1]} \|F(z^{(k)} + \alpha\delta z^{(k)})\|_2$$

   The Armijo rule [6] can be used.

6. Solve for

$$\begin{aligned} p(1)^{(k+1)} &= p(1)^{(k)} + \alpha^{(k)} \delta p(1) \\ \tau^{(k+1)} &= \tau^{(k)} + \alpha^{(k)} \delta \tau \end{aligned}$$

7. Stop if $\|\delta z\|_2 < \xi$ for very small $\xi > 0$, or set $k = k + 1$ and return to step (2).

It is well know that, if the initialization of the shooting parameters are close enough to the exact value, then the Newton method is fast to converge. In order to have a good initialization for the semi-smooth Newton method, we describe a strategy to have a good initial guess of $p(1)^{(0)}$ and $\tau^{(0)}$ in the algorithm. It is achieved by solving a related minimum norm problem, that is, to minimize the mean square error of the control input $u(t)$ for a fixed time horizon τ.

$$\min \quad \int_0^\tau \frac{|u|^2}{2} \, ds$$

In the necessary optimality system, the control for the minimum norm problem is given by

$$u(t) = -B^T p(t)$$

which is differentiable. Hence Newton method can be applied to solve the necessary optimality system directly. The shooting parameter is $z = p(1)$. We take advantage of the fact that, to solve minimum norm problem using Newton method, the initialization of shooting parameter $z = p(1)$ can simply taken as 0 vector in $\mathbb{R}^n$. In other words, minimum norm problem can be solved without random guess of $z = p(1)$.

To solve the related minimum norm problem on a fixed time horizon τ, we also first scale the time horizon from $[0, \tau]$ to $[0, 1]$ by change of variable. After solving the minimum norm problem, we can find the exact costate $\hat{p}(1)$ at scaled time $t = 1$ for minimum norm problem. By scaling the n-dimensional vector $\hat{p}(1)$ through the transversality condition, we are able to have a good initial guess of $p(1)^{(0)}$ for the time optimal control problem.

$$\begin{aligned} \beta &= -\frac{1}{\hat{p}(1)^T (Ax(1) + \hat{u}(1)B)} \\ p(1)^{(0)} &= \beta \hat{p}(1) \end{aligned}$$

Here $\hat{u}(t)$ denotes the control derived from solving minimum norm problem. Hence we are able to reduce the number of shooting parameter to guess from $n + 1$ initially to 1 only, that is τ , for solving time optimal control problem.

A good initialization of τ can be found in the following strategy: pick up τ such that

$$\sup_{t\in[0,1]} |\hat{u}(t)| \text{ close to } 1$$

In summary, the globalization of the Semi-smooth Newton method to solve time optimal control problem can be achieved by solving a related minimum norm problem to give a good initialization of the shooting parameters and the line search method for the damping factor α.

6.4 The Minimum Effort Control Problem

In this section, we study the minimum effort control problem, which is a converse of the time optimal control problem. It addresses a question of how large control needs be so that the target is achieved at a given terminal time T.

Our proposed method is the same as the one applied to solve for time optimal control problem. A regularization problem is formulated and necessary optimality condition is derived by Lagrange multiplier theory. Then semi-smooth Newton method is applied to solve the regularized optimality system. As we have presented the time-optimal control problem for the linear multi-input system in section 6.2, we describe the minimum effort control problem for the bilinear system. The same approach can also be applied to linear system.

Consider the minimum effort control problem for the bilinear multi-input system with fixed time horizon T, prescribed fixed boundary points and constrained control

$$\begin{cases} \min \quad \displaystyle\sum_{i=1}^{m} \frac{1}{2} |\gamma_i|^2 \\ \text{subject to} \quad \dfrac{d}{dt}x(t) = Ax(t) + \displaystyle\sum_{i=1}^{m} u_i(t) B_i x(t), \\ x(0) = x_0, \quad x(T) = x_f, \\ \text{with} \quad |u_i(t)| \le \gamma_i \end{cases} \tag{Pe}$$

where $A \in \mathbb{R}^{n\times n}$, $B_i \in \mathbb{R}^{n\times m}$, $x_0 \in \mathbb{R}^n$, $x_1 \in \mathbb{R}^n$ are given, the control $u_i(t) \in \mathbb{R}$ is measurable. It is assumed that the system is controllable, that is, x_1 can be reached in finite time by an admissible control.

For each control input u_i, the effort is defined to be the maximum norm of u_i, that is

$$\|u_i\| = \sup_{0\le t\le T} |u_i(t)|$$

The total effort to be minimized is the 2-norm of the effort of control $u(t) = \{u_i(t)\}$, $i = 1, \ldots, m$.

$$\min \quad \sum_{i=1}^{m} \frac{1}{2} \|u_i\|^2$$

In general, the control effort can be defined as the q-norm,

$$\min \quad \sum_{i=1}^{m} \frac{1}{q} \|u_i\|^q, \quad q \ge 1$$

Now let us derive the necessary optimality system. By introducing the Lagrange multiplier $p(t)$, $\lambda_i(t)$, for $i = 1, \ldots, m$, we formulate the Lagrange

$$L = \sum_{i=1}^{m} \frac{1}{2} |\gamma_i|^2 + \int_0^T p^T((Ax + \sum_{i=1}^{m} u_i B_i x) - \frac{dx}{dt})\, dt + \int_0^T \lambda_i(t)(|u_i(t)| - \gamma_i)\, dt$$

Take the derivative of L with respect to x and using integration by parts, $\frac{\partial L}{\partial x} = 0$ we have

$$\int_0^1 (A + \sum_{i=1}^{m} u_i B_i)^T p - \frac{\partial}{\partial x}[p^T x|_0^1 - \int_0^1 x^T \frac{dp}{dt}] = 0$$

$$\int_0^1 ((A + \sum_{i=1}^{m} u_i B_i)^T p + \frac{dp}{dt})\, dt = 0$$

hence

$$-\frac{dp(t)}{dt} = (A + \sum_{i=1}^{m} u_i B_i)^T p(t), \tag{6.28}$$

Set $\frac{\partial L}{\partial p} = 0$, we have

$$\frac{dx(t)}{dt} = Ax + \sum_{i=1}^{m} u_i B_i x \tag{6.29}$$

Set $\frac{\partial L}{\partial \gamma_i} = 0$, we have the condition

$$\gamma_i - \int_0^T \lambda_i(t)\, dt = 0 \tag{6.30}$$

Set $\frac{\partial L}{\partial u_i} = 0$, (the Frechet derivative) we have

$$\int_0^T (p^t B_i x, v)\, dt + \int_0^1 \lambda_i(\frac{u_i}{|u_i|}, v)\, dt = 0$$

$$p^t B_i x + \lambda_i \frac{u_i}{|u_i|} = 0$$

hence,

$$\lambda_i(t) = |p^T B_i x| \tag{6.31}$$

$$u_i(t) = -\gamma_i \operatorname{sign}(p^T B_i x) \tag{6.32}$$

In summary, the necessary optimality system for (Pe) is given by

$$\begin{cases} \dot{x} = Ax + \sum_{i=1}^{m} u_i B_i x, \ x(0) = x_0, \ x(T) = x_f, \\ -\dot{p} = (A + \sum_{i=1}^{m} u_i B_i)^T p, \\ u_i(t) = -\gamma_i \operatorname{sign}(p^T B_i x) \\ \gamma_i - \int_0^T |p^T B_i x(t)| \, dt = 0 \end{cases} \tag{6.33}$$

We see that for each control input, $u_i(t)$ is bang-bang, which prohibits the use of Newton-type methods to solve for solving the optimality system (6.33) numerically. Therefore, we consider a family of regularized problems

$$\begin{cases} \min \quad \sum_{i=1}^{m} \frac{1}{2} |\gamma_i|^2 + \int_0^T \frac{\varepsilon}{2} |u_i(t)|^2 \, dt \\ \text{subject to} \quad \frac{d}{dt} x(t) = Ax(t) + \sum_{i=1}^{m} u_i(t) B_i x(t), \\ x(0) = x_0, \quad x(T) = x_f, \\ \text{with} \quad |u_i(t)| \leq \gamma_i \end{cases} \tag{Pe_ε}$$

with $\varepsilon > 0$. As $\varepsilon \to 0$, the cost functional in (Pe_ε) converges to the original cost functional in (Pe). We can prove the convergence of the solutions $(x^\varepsilon, p^\varepsilon, u^\varepsilon, \gamma^\varepsilon)$ of (Pe_ε) to a solution $(x^*, p^*, u^*, \gamma^*)$ of (Pe).

Proposition 6.4.1 *For every $0 < \varepsilon_0 < \varepsilon_1$ and each component $i = 1, \ldots, m$ we have*

$$\gamma_i^* \leq \gamma_i^{\varepsilon_0} \leq \gamma_i^{\varepsilon_1} \leq \gamma_i^* \sqrt{1 + \frac{\varepsilon_1 T}{2}}, \tag{6.34}$$

$$|u_i^{\varepsilon_1}|_{L^2(0,T)} \leq |u_i^{\varepsilon_0}|_{L^2(0,T)} \leq |u_i^*|_{L^2(0,T)}. \tag{6.35}$$

The Proposition (6.4.1) implies the monotonicity of solution (u, γ) with respect to the parameter ε. The following theorem gives the asymptotic properties of solutions of regularized problems.

Theorem 6.4.1 *For $\varepsilon \to 0^+$ we have $\gamma_i^\varepsilon \to \gamma_i^*$ for each $i = 1, \ldots, m$ and every convergent subsequence of solutions $\{(u^\varepsilon,\, x^\varepsilon)\}_{\varepsilon>0}$ of (Pe_ε) converges in $L^2(0,\,T; \mathbb{R}^m) \times W^{1,2}(0,\,T;\,\mathbb{R}^n)$ to a solution $(u^*,\, x^*)$ of (Pe).*

By Lagrange multiplier theory again, the necessary optimality system for (Pe_ε) can be derived. It is given by

$$\begin{cases} \dot{x} = Ax + \displaystyle\sum_{i=1}^{m} u_i B_i x,\ x(0) = x_0,\ x(T) = x_f, \\ -\dot{p} = (A + \displaystyle\sum_{i=1}^{m} u_i B_i)^T p, \\ u_i(t) = -\gamma_i \operatorname{sign}_\varepsilon(p^T B_i x), \\ \gamma_i - \displaystyle\int_0^T |\varepsilon u_i(t) + p^T B_i x(t)|\, dt = 0, \quad i = 1, \ldots, m. \end{cases} \tag{6.36}$$

To solve the regularized optimality system (6.36), we apply the semi-smooth Newton method. A generalized derivative of $\operatorname{sign}_\varepsilon$ is taken as G_ε in (6.22).

6.5 Linear System

In this section, we apply the semismooth Newton method to solve time optimal and minimum effort control problem for the linear system. Several examples are demonstrated to show the effectiveness of our method.

Recall that, we consider the time-optimal control problem of time-invariant linear systems with prescribed fixed boundary points and constrained control.

$$\min \quad \tau = \int_0^\tau 1\, dt \tag{6.37}$$

$$\frac{dx(t)}{dt} = Ax(t) + Bu(t) \tag{6.38}$$

$$x(0) = x_0, x(\tau) = x_f \tag{6.39}$$

$$\text{subject to} \quad |u(t)| \leq \gamma \tag{6.40}$$

It is assumed that $x(t) \in \mathbb{R}^n$ is the state variable, $u(t) \in \mathbb{R}^m$ is the control, $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$. τ is the time a prescribed final state is attained. The admissible control $u(t)$ is bounded above by $\gamma \in \mathbb{R}^n$. The control constraint (6.40) is interpreted as

$$|u_i(t)| \leq \gamma_i \quad \text{for } i = 1, \ldots, m$$

We assume that the system is controllable. The system (6.37)-(6.40) is said to be controllable if for every x_0 and x_f in $\mathbb{R}^n$ and every $t_1 > 0$, there exists a piecewise continuous control $u(t)$ such that if $x(0) = x_0$ then $x(t_1) = x_f$. A necessary and sufficient condition for controllability is that Rank$(B, AB, ..., A^{n-1}B) = n$ where , indicates a column partition.

The following two theorems characterize the existence and uniqueness of control for the linear system, see [15], [37].

Theorem 6.5.1 *If all the eigenvalues of A have nonpositive real parts, and an optimal control exists that transfers any initial state x_0 to the origin. Furthermore, if an extremal control exists, then it is unique.*

Theorem 6.5.2 *If the eigenvalues of A are all real, and a (unique) time-optimal control exists, then each control component can switch at most (n-1) times.*

As described in Section (6.2) and (6.3), a regularized problem is formulated and the semi-smooth Newton method is applied for solving the regularized optimality system

$$\dot{x} = \tau(Ax + Bu),\ x(0) = x_0,\ x(1) = x_f \tag{6.41}$$

$$-\dot{p} = \tau A^T p \tag{6.42}$$

$$u = -\text{sign}_\varepsilon(B^T p) \tag{6.43}$$

$$1 + \frac{\epsilon}{2}|u(1)|^2 + p(1)^T(Ax(1) + Bu(1)) = 0, \tag{6.44}$$

Now, We present the numerical scheme used to solve the regularized optimality system. The time horizon $[0, 1]$ is equally partitioned into n parts with time step size $h = \frac{1}{n}$. Starting with $p(1)$ and τ, the adjoint equation (6.42) is computed backwards by using Crank-Nicolson scheme,

$$-\frac{p_{k+1} - p_k}{\Delta t} = \tau A^T \frac{p_{k+1} + p_k}{2}, \quad k = 1 \ldots n+1$$

$$p_{n+1} = p(1)$$

The control (6.43) is then computed at the middle point of two consecutive costates

$$u_k = -\mathrm{sign}_\epsilon(B^T \frac{p_{k+1} + p_k}{2})$$

The state equation (6.41) can be computed based on

$$\begin{aligned} \frac{x_{k+1} - x_k}{\Delta t} &= \tau(A\frac{x_{k+1} + x_k}{2} + Bu_k), \quad k = 1 \dots n \\ x_1 &= x(0) \end{aligned}$$

Since the time integration of $x(t), p(t)$ are computed using Crank-Nicolson scheme, the residue $F_1, F_2 \sim O(h^2)$. The discretization of the variational equation for δx and δp in (6.24) becomes

$$\begin{aligned} -\frac{\delta p_{k+1} - \delta p_k}{\Delta t} &= \tau A^T \frac{\delta p_{k+1} + \delta p_k}{2} + A^T \frac{p_{k+1} + p_k}{2} \delta\tau + g_k, \\ \delta p_{n+1} &= \delta p(1). \end{aligned}$$

$$\begin{aligned} \frac{\delta x_{k+1} - \delta x_k}{\Delta t} &= \tau A \frac{\delta x_{k+1} + \delta x_k}{2} + (A\frac{x_{k+1} + x_k}{2} + Bu_k)\delta\tau + \tau B \delta u_k + f_k \\ \delta x_1 &= \delta x(0) = 0 \end{aligned}$$

where

$$\delta u_k = -G_\epsilon(B^T \frac{p_{k+1} + p_k}{2}) B^T \frac{\delta p_{k+1} + \delta p_k}{2} + h_k$$

Following by [19], the above scheme is consistent and of second order convergence. Set the shooting parameters $z = (p(1), \tau)$. Evaluating the shooting function $F(z)$ and compute the Newton update based on (6.27), the time optimal control problem can be solved in this discretization.

We demonstrate the effectiveness of our semismooth Newton method by the following examples. We start with the simplest case.

Example 1:(Rocket sled problem)

Let $y(t)$ be the displacement of a sled with mass=1 on a friction free surface controlled by an applied force $u(t)$ with constraint $|u(t)| \leq 1$. By Newton's second law of motion, we have

$$\frac{d^2}{dt^2} y(t) = u(t) \tag{6.45}$$

If we defined $x_1(t) = y(t)$ and $x_2(t) = \frac{d}{dt}y(t)$, then the state $x(t) = (x_1(t), x_2(t))^T$ satisfies the linear system (6.38) with

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

We consider the problem to construct a control $u(t)$ that bring the sled to rest in minimum time: $x(\tau) = (0,0)^T$. We observe the eigenvalues of A are both zero, so a unique optimal control exists, and has at most one switching followed by Theorem 6.5.1 and 6.5.2. From the above discussion it follows that u^* must satisfy

$$u^*(t) = -\text{sign}(p_2(t))$$

The adjoint equation implies that $p = (p_1(t), p_2(t))$ is given by

$$p_1(t) = \mu_1 \quad \text{and} \quad p_2(t) = \mu_1(\tau - t) + \mu_2$$

for some nonzero $\mu = (\mu_1, \mu_2)$. Here the costate $p_2(t)$ is a linear function in t, once it is zero, the control need to switch sign. The orbit of the trajectory is a family of parabola.

$$\begin{aligned} x_1(t) &= \frac{1}{2}x_2^2(t) + c_1, \quad \text{for} \quad u = 1 \\ x_1(t) &= -\frac{1}{2}x_2^2(t) + c_2, \quad \text{for} \quad u = -1 \end{aligned}$$

The optimal control u^* is given in feedback form

$$u^*(t) = \eta(x(t)) = \begin{cases} -1, & \text{if } (x_1, x_2) \text{ is above } S; \\ 1, & \text{if } (x_1, x_2) \text{ is below } S. \end{cases}$$

where S is the switching curve in form of $x_1(t) = -\frac{1}{2}x_2(t)|x_2(t)|$.

In the simulation, we take the time step size $h = 10^{-3}$, $\epsilon = 10^{-3}$ for the Yosida approximation sign_ε. The time optimal solution for some initial points are shown in Table 6.1. With a relative good guess of $\tau^{(0)}$, our semi-smooth Newton method gives superlinear convergence. Figure 6.1, 6.2 shows the trajectory and control for the rocket sled problem from $x_0 = [1, 1]$, $x_0 = [-1, -2]$ to the origin. We observe that it has at most one switch in the control input, which agrees with the result in Theorem 6.5.2.

Table 6.1: Numerical solution of time optimal τ for the rocket sled problem

Initial point $x(0)$	Initial guess of $\tau^{(0)}$	exact τ	exact adjoint $p(1)$
$(1;1)$	10	3.4497	(0.2367;-0.2899)
$(-1;-2)$	10	5.4645	(-0.1061;0.1830)
$(5;-2)$	1	3.2916	(0.1147; -0.3038)
$(10;-10)$	35	22.6508	(-0.0070; 0.0441)
$(60;60)$	200	146.566	(0.0002;-0.0068)

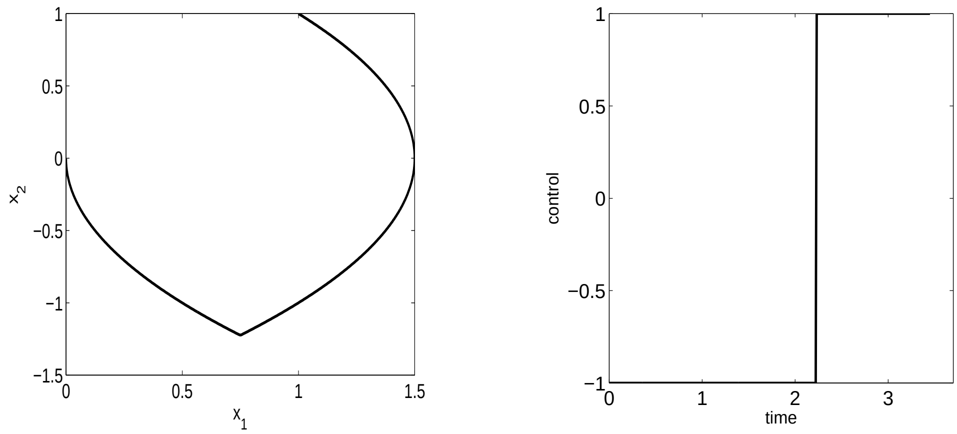

Figure 6.1: The trajectory and control from $x_0 = [1,1]$ to $x_f = [0,0]$ for rocket sled problem, the time optimal $\tau = 3.4497$.

Example 2:(Harmonic oscillator)

We consider the following dynamics for the spring-mass system, known as harmonic oscillator.

$$m\frac{d^2x(t)}{dt^2} + kx(t) = u(t) \tag{6.46}$$

where m is the mass, k is the spring constant. For simplicity, we set $m = 1$, $k = 1$. The control $u(t)$ is interpreted as an exterior force acting on an oscillating weight hanging from a spring. The goal is to design an optimal exterior forcing $u(t)$ that brings the motion to a stop $(x(t) = 0)$ in minimum time.

The system is in the form of (6.38) with

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

In this case, the eigenvalues of A are $\pm i$, hence Theorem 6.5.2 cannot apply, there may exist

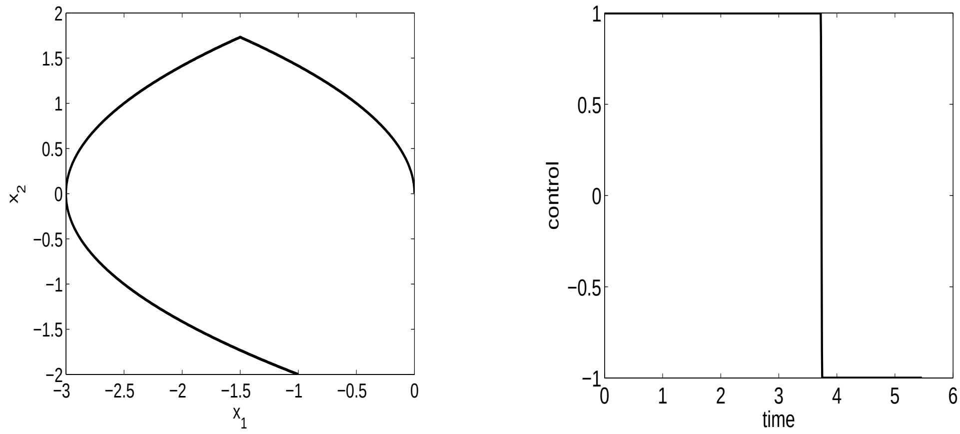

Figure 6.2: The trajectory and control from $x_0 = [-1, -2]$ to $x_f = [0, 0]$ for rocket sled problem, the time optimal $\tau = 5.4645$.

more than one switching in the control. Actually the dynamics of the controlled system are two families of circle with differen radius and centering. If the circles intercept, a switch may be taken. When $u = 1$, the system becomes

$$\frac{dx_1(t)}{dt} = x_2(t)$$
$$\frac{dx_2(t)}{dt} = -x_1(t) + 1$$

note that,

$$\frac{d}{dt}(x_1 - 1)^2 + x_2^2) = 2(x_1 - 1)\frac{dx_1}{dt} + 2x_2\frac{dx_2}{dt} = 0$$

so the trajectory satisfies $(x_1 - 1)^2 + x_2^2 = r_1^2$ for some radius r_1, which is a circle with center $(1, 0)$. Similarly, when $u = -1$, we have the trajectory satisfies $(x_1 + 1)^2 + x_2^2 = r_2^2$ for some radius r_2, which is a circle with center $(-1, 0)$.

The time optimal solution for some initial points are shown in Table 6.2. Figure 6.3 shows the trajectory and control from $x_0 = [-15, 20]$ to $x_f = [0, 0]$ for the harmonic oscillator problem. We observe that, it requires more switchings in the control and longer time to reach the origin if the initial point is far away from the origin. Comparing to the time optimal solution, Figure 6.4 shows the trajectory and control for the minimum norm solution from $x_0 = [-15, 20]$ to $x_f = [0, 0]$ on a fixed time horizon $T = 40$. We see that the trajectory for both cases are similar, but the control are different. The control for minimum norm solution is continuous and differentiable, while the control for time optimal solution is bang-bang.

Table 6.2: Numerical solution of time optimal τ for the harmonic oscillator problem

Initial point $x(0)$	initial guess on $\tau^{(0)}$	exact τ	exact adjoint $p(1)$
$(1;1)$	1	2.4982	(0.0008; -0.4003)
$(4;-2)$	3	6.9858	(0.0846; -0.1431)
$(10;-10)$	16	22.2081	(-0.0311; 0.0450)
$(-15;20)$	30	38.7655	(0.0113; 0.0258)

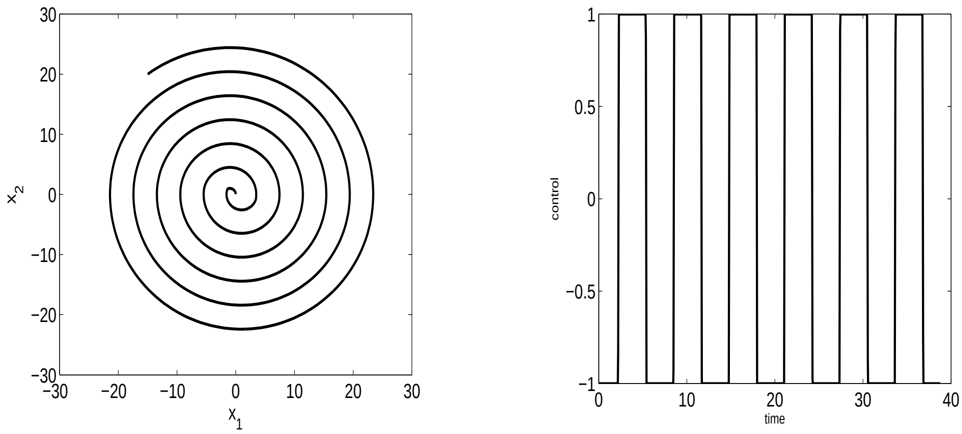

Figure 6.3: The trajectory and control for the time optimal solution from $x_0 = [-15, 20]$ to $x_f = [0, 0]$ of harmonic oscillator problem, $\tau = 38.7655$

Example 3:(Spacecraft)

The following example is studied in [8] [5]. We consider the single-axis slew maneuvers of simple flexible spacecraft, consisting of a rigid hub and flexible appendages. A discrete model for this problem can be obtained by the assumed modes methods. In state space, with two modes (one rigid and one flexible), we obtain the linear system (6.38) with

$$A = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -\omega^2 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 \\ g_0 \\ 0 \\ g_1 \end{pmatrix}$$

where ω is the fundamental frequency. We consider rest-to-rest maneuvers. For this case, the initial condition is given by

$$x_0 = [-\theta, 0, 0, 0]^T$$

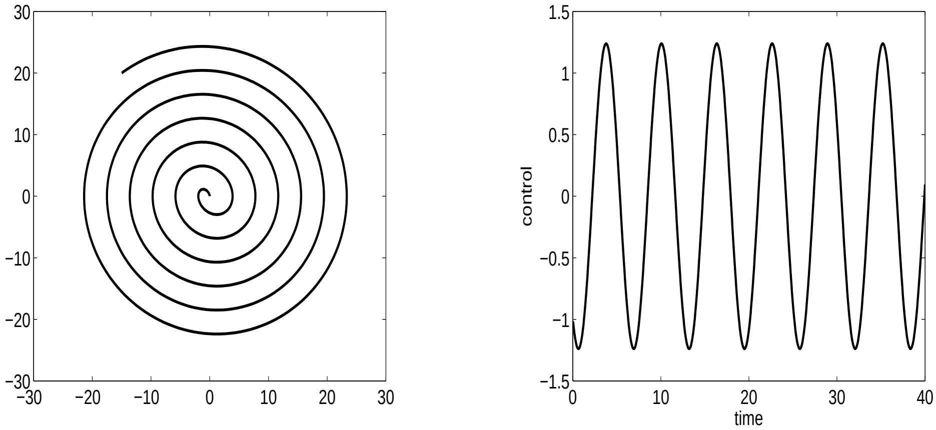

Figure 6.4: The trajectory and control for the minimum norm solution from $x_0 = [-15, 20]$ to $x_f = [0, 0]$ of harmonic oscillator problem for a fixed horizon $T = 40$

and the final state x_f is the zero vector. We solve this problem with the following numerical values: $\theta = 15$, $\omega = 3.0904$, $g_0 = 0.0226$ and $g_1 = 0.00218$.

For the minimum norm problem, The control input $u(t)$ is unconstrained. For a fixed time horizon $T = 2.5$, Figure 6.5 shows the resulting trajectory and control.

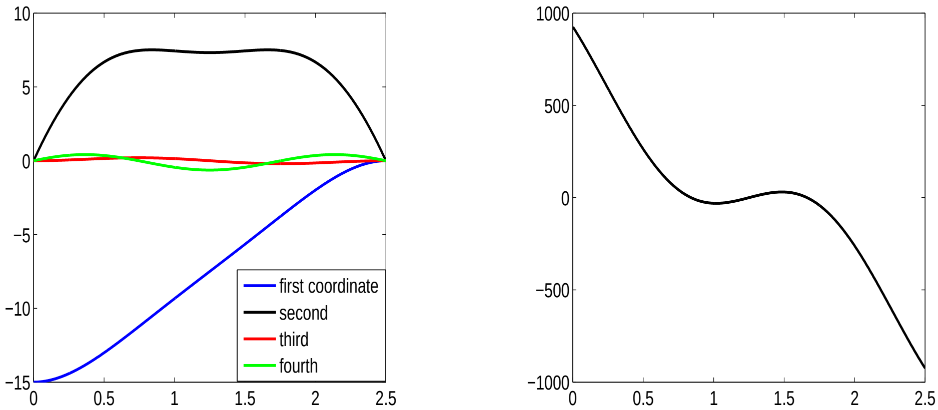

Figure 6.5: The trajectory and control of minimum norm solution for the control of spacecraft with the fixed time horizon $T = 2.5$

For time optimal control problem, the control $u(t)$ is bounded above by γ, $|u(t)| \leq \gamma$. With different γ, Table 6.3 shows the resulting time optimal solution τ. We see there are 3 switchings in the control. Figure 6.6 shows the resulting trajectory and control. Comparing to the trajectory of minimum norm solution, we observe that the first coordinate of the state $x(t)$ becomes shaper and shaper with smaller γ.

Table 6.3: Numerical solution of time optimal τ for the control of a spacecraft with different control magnitude γ

γ	time optimal τ	number of switch
50	7.3281	3
100	5.2670	3
200	3.6651	3
500	2.6253	3
600	2.4881	3

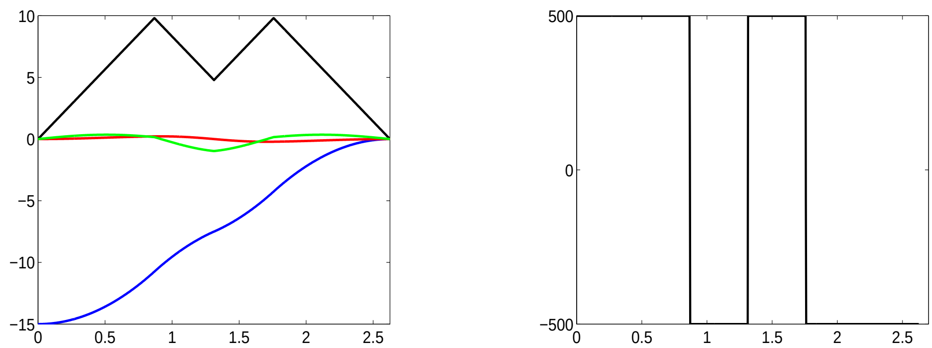

Figure 6.6: The trajectory and control of time optimal control problem for the control of spacecraft, the minimum time $\tau = 2.6253$

For the minimum effort problem with a fixed horizon T, suppose $|u(t)| \leq \gamma$, the cost functional to be minimized is γ. With different horizon T, Table 6.4 shows the resulting minimum effort γ. We see there are 3 switchings in the control. Figure 6.7 shows the resulting trajectory and control for the minimum effort problem.

Another interesting simulation we have done is for minimum effort problem with two controls. Previously, the control potential B includes g_0, g_1 in the second and fourth coordinate. Hence it is natural to include another control potential which can control the first and third coordinate. The problem can be stated as

$$\frac{dx(t)}{dt} = Ax(t) + u_1(t)B_1 + u_2(t)B_2$$

Table 6.4: Numerical solution of minimum effort γ for the control of a spacecraft with different time horizon T

T	minimum γ	number of switch
2	1372.1	3
2.5	590.1336	3
3	331.7338	3
10	27.0980	3

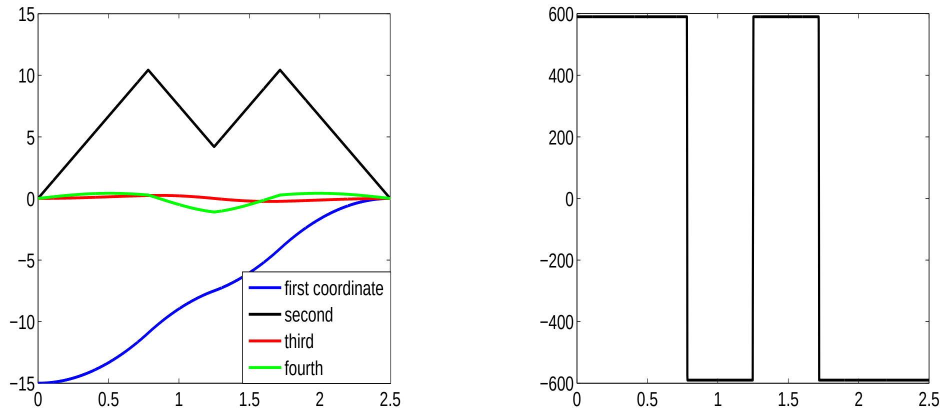

Figure 6.7: The trajectory and control of minimum effort problem for the control of spacecraft, the minimum effort $\gamma = 590.1336$

with

$$B1 = [0, g_0, 0, g_1]^T, \quad B2 = [g_2, 0, g_3, 0]^T$$

here we set $g_2 = 0.02$, $g_3 = 0.01$. With the constrained control $|u_1(t)| \leq \gamma_1$, $|u_2(t)| \leq \gamma_2$, we focus on minimizing the cost functional

$$\min \quad \frac{1}{2}(\gamma_1^2 + \gamma_2^2)$$

For fixed time horizon $T = 2.5$, the minimum control effort is given by

$$\gamma_{\text{opt}} = \begin{pmatrix} 179.9036 \\ 201.7777 \end{pmatrix}$$

Figure 6.8 shows the the control u_1 has one switching while control u_2 has four switchings.

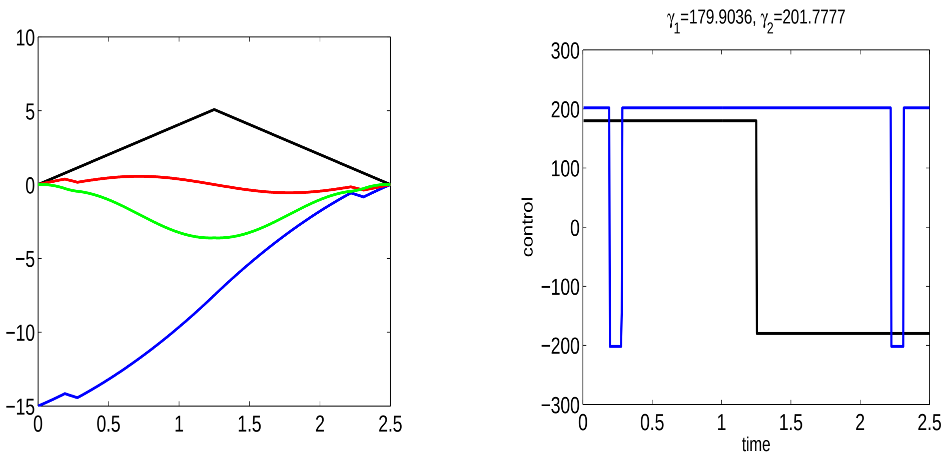

Figure 6.8: The trajectory and control of minimum effort problem for the control of space-craft with two control potentials

6.6 Bilinear System

In this section, we apply the semi-smooth Newton method to solve the time optimal control problem for bilinear system. Several examples are demonstrated to show the effectiveness of our method.

We consider the time-optimal control problem of time-invariant bilinear systems with prescribed fixed boundary points and constrained control.

$$\min \quad \tau = \int_0^\tau 1\, dt \tag{6.47}$$

$$\frac{dx(t)}{dt} = Ax(t) + \sum_{i=1}^{m} B_i u_i(t) x(t) \tag{6.48}$$

$$x(0) = x_0,\ x(\tau) = x_f \tag{6.49}$$

$$\text{subject to} \quad |u_i(t)| \le \gamma_i, \quad i = 1, \ldots, m \tag{6.50}$$

It is assumed that $x(t) \in \mathbb{R}^n$, $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times n}$. τ is the time when a prescribed final state is attained. The admissible control $u_i(t) \in \mathbb{R}$ is bounded above by γ_i. For simplicity, we set number of control $m = 1$. We assume the system (A, B) is controllable. The result on controllability of bilinear system can be found in [9].

Similar to the time optimal control on linear system, the time horizon is first scaled from $[0, \tau]$ to $[0, 1]$ by change of variable. The Hamiltonian of the system is

$$H(x, p, u) = \tau + \tau p^T (Ax + Bux)$$

Derived from the optimality system (6.5)-(6.10), the necessary optimality for time optimal control problem on bilinear system becomes

$$\frac{dx(t)}{dt} = H_p = \tau(Ax(t) + u(t)Bx(t)) \tag{6.51}$$

$$-\frac{dp(t)}{dt} = H_x = \tau(A + u(t)B)^T p(t) \tag{6.52}$$

$$u(t) = -\gamma \text{sign}(p(t)^T Bx) \tag{6.53}$$

$$1 + \tau p(1)^T (A + Bu(1))x(1) = 0 \tag{6.54}$$

$$x(0) = x_0, x(1) = x_f. \tag{6.55}$$

In the transversality condition (6.54), we artificially add τ to increase the speed of convergence of Newton method, because the control $u(t)$ consists of sign function, which does not depend on the scale of costate $p(t)$. Another advantage of doing this is related to the proposed backward shooting technique, which will be described later.

A regularized problem is formulated to minimize the cost functional

$$\min_{\tau \geq 0} \int_0^\tau (1 + \frac{\varepsilon}{2} |u(s)|^2) \, ds$$

The regularized optimality system is given by

$$\begin{cases} \dot{x} = \tau(Ax + uBx), \; x(0) = x_0, \; x(1) = x_1 \\ -\dot{p} = \tau(A + uB)^T p \\ u = -\text{sign}_\varepsilon(p^T Bx) \\ 1 + \frac{\epsilon}{2}|u(1)|^2 + \tau p(1)^T (Ax(1) + u(1)Bx(1)) = 0, \end{cases} \tag{6.56}$$

We apply the semi-smooth Newton method is solve the necessary optimality system (6.56). To compute reduced Jacobian with some shooting parameters, here we present two types of shooting for the Newton method. Their difference is on the choice of shooting parameters and shooting functions. The first one is called forward shooting where the shooting parameter $z = (p(0), \tau)$, and the shooting function is

$$F(z) = \begin{pmatrix} 1 + \frac{\epsilon}{2}|u(1)|^2 + \tau p(1)^T (Ax(1) + u(1)Bx(1)) \\ x(1) - x_f \end{pmatrix}$$

With an initial guess of z^0, we can solve the initial value problem for $x(t)$ and $p(t)$ to evaluate the shooting function $F(z)$. The Jacobian of the semi-smooth Newton method is computed based on the following variation.

$$\frac{d\delta x}{dt} = \tau(A+uB)\delta x + (A+uB)x\delta\tau + \tau Bx\delta u + f \tag{6.57}$$

$$-\frac{d\delta p}{dt} = \tau(A+uB)^T\delta p + (A+uB)^T p\delta\tau + \tau B^T p\delta u + g \tag{6.58}$$

$$\delta u = -G_\epsilon(p^T Bx)[p^T B\delta x + (Bx)^T\delta p] + h \tag{6.59}$$

where f, g are the errors resulting from the time integration of state $x(t)$ and costate $p(t)$, h is the error from the evaluation of control $u(t)$. The equation (6.57) and (6.58) can be solved as a system,

$$\frac{d}{dt}\begin{pmatrix} \delta x(t) \\ -\delta p(t) \end{pmatrix} = \tau \begin{pmatrix} A+uB-G_\epsilon Bxp^T B & -G_\epsilon(p^T Bx)Bx(Bx)^T \\ G_\epsilon(p^T Bx)B^T pp^T B & (A+uB)^T - G_\epsilon B^T p(Bx)^T \end{pmatrix}\begin{pmatrix} \delta x(t) \\ \delta p(t) \end{pmatrix} + \begin{pmatrix} (A+uB)x \\ (A+uB)^T p \end{pmatrix}\delta\tau + \begin{pmatrix} f+\tau Bxh \\ g+\tau B^T ph \end{pmatrix} \tag{6.60}$$

After Integrating (6.60), we have $\delta x(1)$, $\delta p(1)$ as a function of $\delta p(0)$ and $\delta\tau$. The variations on the shooting function are

$$\delta x(1) + x(1) - x_f = 0$$

$$\epsilon u(1)\delta u(1) + \tau[(A+u(1)B)x(1)]^T\delta p(1) + \tau p(1)^T(A+u(1)B)\delta x(1) \\ +\tau p(1)^T Bx(1)\delta u(1) + p(1)^T(A+Bu(1))x(1)\delta\tau + l = 0$$

where $l = 1 + \frac{\epsilon}{2}|u(1)|^2 + \tau p(1)^T(A+u(1)B)x(1)$. Hence we can formulate the reduced form of semi-smooth Newton iteration, that is,

$$J\begin{pmatrix} \delta p(0) \\ \delta\tau \end{pmatrix} = \begin{pmatrix} r_1 \\ r_2 \end{pmatrix}.$$

where $J \in \mathbb{R}^{(n+1)\times(n+1)}$.

The second shooting is called backward shooting, where the shooting parameter is $z = p(1)$, the shooting function is $F(z) = x(0) - x_0$. Comparing with the forward shooting method, the backward shooting method reduce the dimension of shooting parameter from

$n+1$ to n. By utilizing the transversality condition (6.54), we are able to eliminate τ with a initial guess of $p(1)$ by using the transversality condition. This is another advantage why we artificially introduce τ into the transversality condition.

$$\tau = -\frac{1}{p(1)^T[(A+u(1)B)x(1)]} \tag{6.61}$$

$$\frac{\partial\tau}{\partial p(1)} = -\frac{(A+u(1)B)x(1)}{(p(1)^T[(A+u(1)B)x(1)])^2} \tag{6.62}$$

Integrating the state and costate equation (6.51) (6.52) backwards, we can evaluate the shooting function $F(z)$. After Integrating (6.60) backwards starting with $\delta x(1) = 0$, we get

$$\begin{aligned} \delta x(0) &= C\delta p(1) + D\delta\tau + E \\ &= (C + D\frac{\partial\tau}{\partial p(1)})\delta p(1) + E \end{aligned}$$

for some $C \in \mathbb{R}^{n\times n}, D \in \mathbb{R}^n, E \in \mathbb{R}^n$. The update on $p(1)$ can be computed by the variation on $F(z)$,

$$(C + D\frac{\partial\tau}{\partial p(1)})\delta p(1) + E + x(0) - x_0 = 0 \tag{6.63}$$

$$\delta p(1) = -(C + D\frac{\partial\tau}{\partial p(1)})^{-1}(x(0) - x_0 + E) \tag{6.64}$$

Now we present the numerical scheme used to solve time optimal control problem for bilinear system by backward shooting. The time horizon $[0,1]$ is equally partitioned into n parts with time step size $h = \frac{1}{n}$. Starting with an initialization of $p(1)$ from solving minimum norm problem, state equation (6.51) and costate equation (6.52) are integrated backwards using Crank-Nicolson scheme, the control is evaluated at left end point.

$$\begin{aligned} \frac{x_{k+1} - x_k}{\Delta t} &= \tau(A + u_k B)\frac{x_{k+1} + x_k}{2}, \quad x_{n+1} = x_f \\ -\frac{p_{k+1} - p_k}{\Delta t} &= \tau(A + u_k B)^T\frac{p_{k+1} + p_k}{2}, \quad p_{n+1} = p(1) \\ u_k &= -sign_\epsilon(Bx_{k+1}, p_{k+1}), \quad k = 1\ldots n \end{aligned}$$

The discretization of the variational equation (6.57)-(6.59) becomes

$$\frac{\delta x_{k+1} - \delta x_k}{\Delta t} = \tau(A + u_k B)\frac{\delta x_k + \delta x_{k+1}}{2} + (A + u_k B)^T\frac{x_{k+1} + x_k}{2}\delta\tau + \tau B\frac{x_{k+1} + x_k}{2}\delta u_k$$

$$\delta x_{n+1} = \delta x(1) = 0$$

$$-\frac{\delta p_{k+1} - \delta p_k}{\Delta t} = \tau (A + u_k B)^T \frac{\delta p_k + \delta p_{k+1}}{2} + (A + u_k B)^T \frac{p_{k+1} + p_k}{2} \delta\tau + \tau B^T \frac{p_{k+1} + p_k}{2} \delta u_k$$

$$\delta p_{n+1} = \delta p(1)$$

$$\delta u_k = -G_\epsilon (B x_{k+1}, p_{k+1})(p_{k+1}^T B \delta x_{k+1} + (B x_{k+1})^T \delta p_{k+1}))$$

Next, We demonstrate the effectiveness of the semismooth Newton method to solve time optimal control problem by the following examples of bilinear systems.

Example 1:(Parabola and circle)

We consider the following bilinear system whose families of trajectories are parabola and circle. The dynamics of the system satisfies

$$\frac{d^2 x(t)}{dt^2} - u(t)x(t) = 0 \tag{6.65}$$

then the state $x(t) = (x_1(t), x_2(t))^T$ satisfies the bilinear system (6.48) with

$$A = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}$$

when the control $u = 1$, we have

$$\frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

The eigenvalue of the matrix is $\lambda = \pm 1$, so

$$x_1 = c_1 e^t + c_2 e^{-t}$$
$$x_2 = c_1 e^t - c_2 e^{-t}$$

The trajectory is a family of hyperbolas satisfying $x_1^2 - x_2^2 = 4c_1c_2$. The asymptotic lines are $x_1 = \pm x_2$, which divide the Cartesian plane into 8 directional fields along with the x and y axis.

When the control is $u = -1$, we have

$$\frac{d}{dt} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

The eigenvalue of the matrix is $\lambda = \pm i$, so

$$x_1 = c_1 \cos(t) + c_2 \sin(t)$$
$$x_2 = -c_1 \sin(t) + c_2 \cos(t)$$

The trajectory is a a family of circles satisfying $x_1^2 + x_2^2 = c_1^2 + c_2^2$.

The numerical simulation is tested for cases where the initial point $x(0) = [1; 1]^T$, Table 6.5 shows some of the time optimal solution for different target points. Figure 6.9 shows a typical trajectory and control pattern.

Table 6.5: Numerical solution of time optimal τ for bilinear system with parabola and circle trajectories

Target	initial guess of τ	exact τ	exact adjoint $p(1)$
$(0.5; -0.5)$	1	2.2639	(0.5524; -0.3310)
$(0; -0.5)$	1	3.0178	(0.5524; -0.3310)
$(0; 0.5)$	4	5.9885	(-0.3340; 0.2325)
$(2; 4)$	4	6.5845	(-0.0290; -0.0180)
$(2; -4)$	2	3.0438	(0.0328; 0.0988)

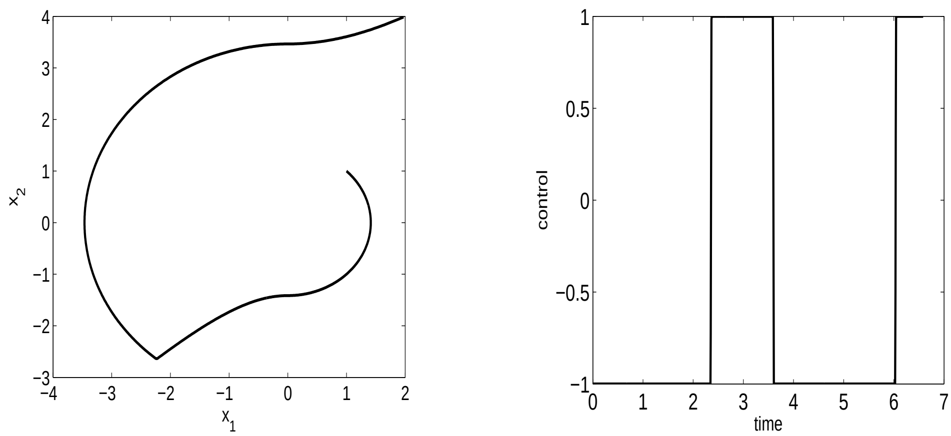

Figure 6.9: The trajectory and control from $x_0 = [1, 1]$ to $x_f = [2, 4]$ for the parabola and circle case, the time optimal $\tau = 6.5845$

Example 2:(Ellipse)

We consider the following bilinear system whose families of trajectories are ellipses. The dynamics of the system satisfies

$$\frac{d^2x(t)}{dt^2} + (1 - \frac{u(t)}{2})x(t) = 0 \tag{6.66}$$

then the state $x(t) = (x_1(t), x_2(t))^T$ satisfies the bilinear system (6.48) with

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ \frac{1}{2} & 0 \end{pmatrix}$$

when we take the control $u = 1$, we have

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{1}{2} & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

The eigenvalue of the matrix is $\lambda = \pm\sqrt{\frac{1}{2}}i$, the parametric form is

$$\begin{aligned} x_1(t) &= c_1 \cos(\sqrt{\frac{1}{2}}t) + c_2 \sin(\sqrt{\frac{1}{2}}t) \\ x_2(t) &= c_1\sqrt{\frac{1}{2}} \sin(\sqrt{\frac{1}{2}}t) + c_2\sqrt{\frac{1}{2}} \cos(\sqrt{\frac{1}{2}}t) \end{aligned}$$

So the trajectory of the system is a family of ellipsis in the form of $x_1^2 + \frac{x_2^2}{\frac{1}{2}} = r_1$, where r_1 is some positive constant. Similarly, when we take the control $u = -1$, we have

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\frac{3}{2} & 0 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

The eigenvalue of the matrix is $\lambda = \pm\sqrt{\frac{3}{2}}i$, the trajectory of the system is a family of ellipsis in the form of $x_1^2 + \frac{x_2^2}{\frac{3}{2}} = r_2$, where r_2 is some constant.

In summary, the trajectory of the controlled system is families of ellipsis centering at origin with different major axis and minor axis. There are also two cases to be considered: (1) $\|x_0\| < \|x_f\|$ or (2) $\|x_0\| > \|x_f\|$. In order to reach the terminal point, we must switch our control $u(t)$ back and forth between the values ± 1 to make the trajectory to switch between different ellipsis in order to decrease or increase the radius.

The numerical simulation is tested for cases where the initial point $x(0) = [1, 1]^T$, Table 6.6 shows some of the time optimal solution for different target points. Figure 6.10 shows a typical trajectory and control pattern. As we observe, the target point

Table 6.6: Numerical solution of time optimal τ for bilinear system with ellipse trajectories

Target	initial guess of τ^0	exact τ	exact adjoint $p(1)$	number of switchings
$(0.5; 0.5)$	3	5.6417	(0.1602; 0.3432)	4
$(0.3; 0.3)$	5	11.0478	(0.0980; 0.2665)	8
$(0.1; 0.1)$	13	17.2707	(0.3878; 0.6445)	12
$(4; 4)$	9	11.2841	(-0.0257;-0.0072)	8

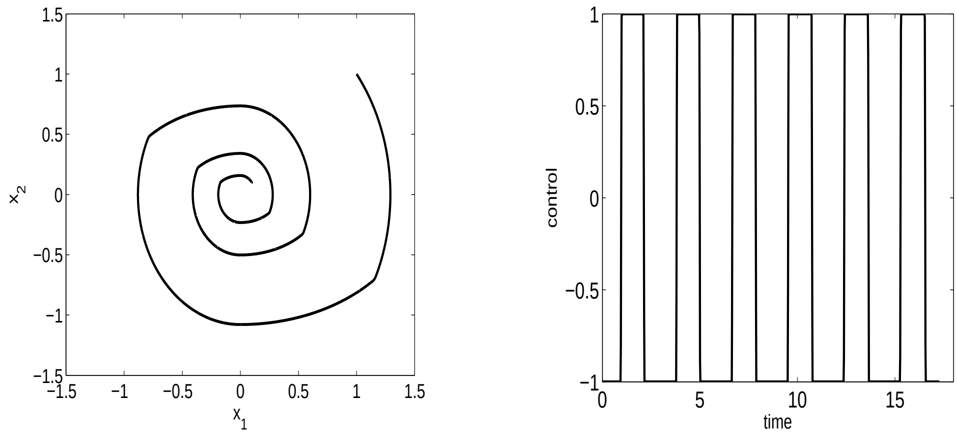

Figure 6.10: The trajectory and control from $x_0 = [1, 1]$ to $x_f = [0.1, 0.1]$ for the ellipse case, the time optimal $\tau = 17.270$

$x_f = [0.1, 0.1]^T$ is very close to the origin, it takes 3 windings to get there, and there are 12 switchings in the control.

Example 3:(Spiral)

We consider the following bilinear system whose families of trajectories are spirals. The dynamics of the system satisfies

$$\frac{d^2x(t)}{dt^2} + u(t)\frac{dx(t)}{dt} + x(t) = 0 \tag{6.67}$$

then the state $x(t) = (x_1(t), x_2(t))^T$ satisfies the bilinear system (6.48) with

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad B = \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix}$$

when we take the control $u = 1$, we have

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & -1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

Table 6.7: Numerical solution of time optimal τ for bilinear system with spiral shape

Target	initial guess of τ	exact τ	exact adjoint $p(1)$	number of switching
$(0; -0.5)$	2	2.5134	(-0.1219; -0.9177)	2
$(0.7; 0.5)$	10	4.9731	(-0.0676;0.1394)	4
$(0; -0.2)$	6	7.1715	(0.3895;-0.3077)	6
$(0; 0.1)$	5	9.7015	(-0.5934; 0.4373)	8

The eigenvalue of the matrix is $\lambda = \frac{-1\pm\sqrt{3}i}{2}$, hence this is a family of trajectories decaying to the origin as $t \to \infty$.

When we take the control $u = -1$, we have

$$\frac{d}{dt}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$$

The eigenvalue of the matrix is $\lambda = \frac{1\pm\sqrt{3}i}{2}$, hence this is a family of trajectories blowing up. Since $u(t) = \text{sign}(x_2(t)p_2(t))$, a switching will occur when the trajectory intersects with the x-axis. The numerical simulation is tested for cases where the initial point $x(0) = [1, 1]^T$, Table 6.7 shows some of the time optimal solution for different target points. Figure 6.11 and Figure 6.12 show some typical trajectories and control patterns.

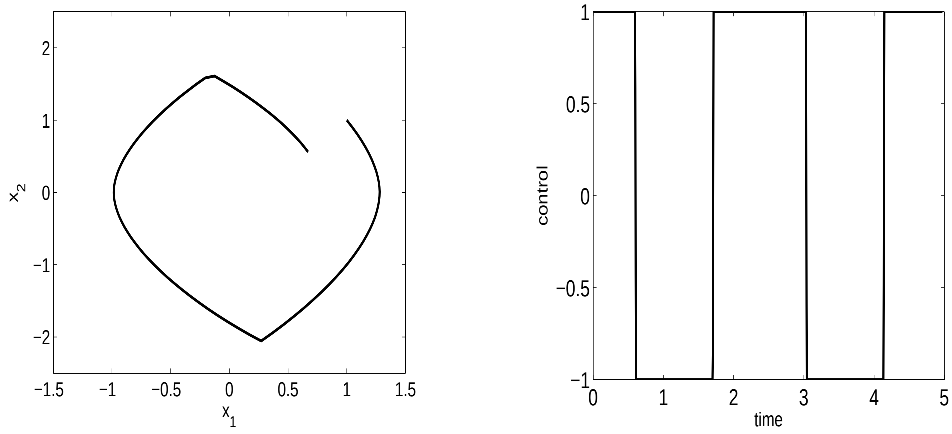

Figure 6.11: The trajectory and control from $x_0 = [1, 1]$ to $x_f = [0.7, 0.5]$ for the spiral case, the time optimal $\tau = 4.9731$

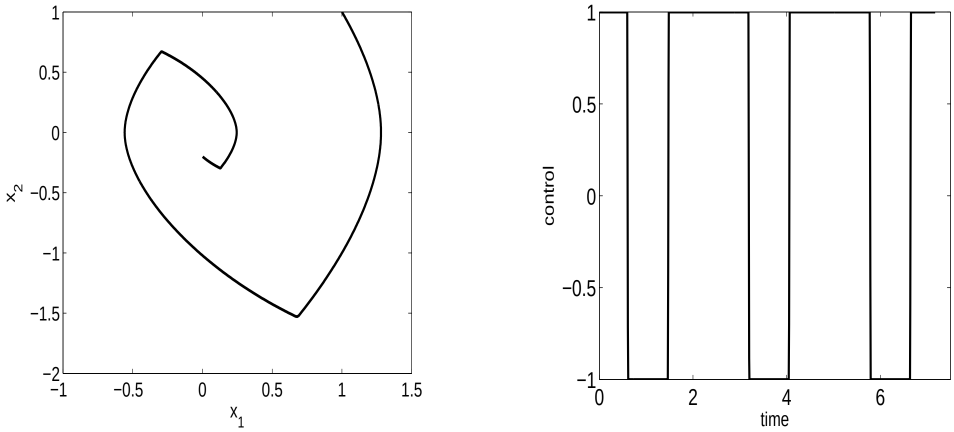

Figure 6.12: The trajectory and control from $x_0 = [1, 1]$ to $x_f = [0, -0.2]$ for the spiral case, the time optimal $\tau = 7.1715$

6.7 Control on Spin-$\frac{1}{2}$ system

Time optimal control problem on quantum spin system has received considerable investigation recently, see [35] [73]. In this section, we apply the regularization process and the semi-smooth Newton method describe in section 6.2 and 6.3 to solve time optimal and minimum effort control problem for quantum spin system.

In closed quantum mechanics, the time evolution of the state vector of a quantum system is described by the time-dependent Schrödinger equation,

$$i\frac{d}{dt}\Psi(x,t) = (\mathcal{H}_0 + \epsilon(t)V)\Psi(x,t) \tag{6.68}$$

Recall from the Introduction section, the dynamics of a typical two-state system, for instance, spin-$\frac{1}{2}$ system, satisfies

$$i\frac{d}{dt}\Psi(x,t) = \frac{1}{2}(\sigma_z + \sigma_x\epsilon_x(t) + \sigma_y\epsilon_y(t))\Psi(x,t) \tag{6.69}$$

where σ_x, σ_y, σ_z are Pauli matrices (1.4). The state vector $\Psi(x,t) \in \mathbb{C}^2$ can be rewritten as $\Psi = \Psi_1 + i\Psi_2$, then (6.69) is equivalent as

$$\frac{d}{dt}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} = \begin{pmatrix}0 & I_z\\ -I_z & 0\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} + \epsilon_x(t)\begin{pmatrix}0 & I_x\\ -I_x & 0\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} + \epsilon_y(t)\begin{pmatrix}0 & I_y\\ -I_y & 0\end{pmatrix}\begin{pmatrix}\Psi_1\\ \Psi_2\end{pmatrix} \tag{6.70}$$

where $I_z = \frac{1}{2}\sigma_z$, $I_x = \frac{1}{2}\sigma_x$, $I_y = \frac{1}{2}\sigma_y$.

The control problem is stated as to find the control inputs $\epsilon_x(t)$, $\epsilon_y(t)$ to drive the quantum system from initial state $\Psi(0) \in \mathbb{C}^2$ with $\|\Psi(0)\|_2 = 1$ to the ground state $|g\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$. For simplicity, we consider the case where only control input $\epsilon_x(t)$ is active.

$$\frac{d}{dt}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} = \begin{pmatrix} 0 & I_z \\ -I_z & 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} + \epsilon_x(t)\begin{pmatrix} 0 & I_x \\ -I_x & 0 \end{pmatrix}\begin{pmatrix} \Psi_1 \\ \Psi_2 \end{pmatrix} \tag{6.71}$$

Let $x(t) = [\Psi_1, \Psi_2]^T \in \mathbb{R}^4$, then we have a real-valued bilinear system

$$\frac{dx(t)}{dt} = Ax(t) + u(t)Bx(t) \tag{6.72}$$

with $A = \begin{pmatrix} 0 & I_z \\ -I_z & 0 \end{pmatrix}$, $B = \begin{pmatrix} 0 & I_x \\ -I_x & 0 \end{pmatrix}$, $u(t) = \epsilon_x(t)$ is the admissible control. The state $x(t)$ is normalized in Euclidean norm. The ground state is in the form of $\mathcal{O} = [1, 0, 0, 0]^T$.

For minimum norm control problem, the control objective is to minimize

$$\min \quad \int_0^T \frac{|u|^2}{2}\, dt$$

for a fixed horizon T. It is used as the initialization process to get a reasonable guess of the shooting parameters needed for the time optimal and minimum effort control problem. Figure 6.13 shows the the trajectory and control from the state $|\Psi\rangle = \frac{1}{\sqrt{2}}[1, i]^T$ to the ground state $|g\rangle$ on a fixed time horizon $T = 1$ for the minimum norm problem. Here $|\Psi\rangle = \frac{1}{\sqrt{2}}[1, i]^T$ can be equivalently written in real form as $x = \frac{1}{\sqrt{2}}[1, 0, 0, 1]^T$.

For the time optimal control problem, given the maximum control input γ satisfying $|u(t)| \leq \gamma$, we want to find the minimum time τ such that $\Psi(\tau)$ lies on the δ-neighborhood of the ground state $\mathcal{O}$,

$$\frac{1}{2}|\Psi(\tau) - \mathcal{O}|^2 = \delta \tag{6.73}$$

for given small $\delta > 0$. Since $\Psi(0)$ and $\mathcal{O}$ are normalized, (6.73) is equivalent as

$$(\Psi(\tau), \mathcal{O}) = 1 - \delta$$

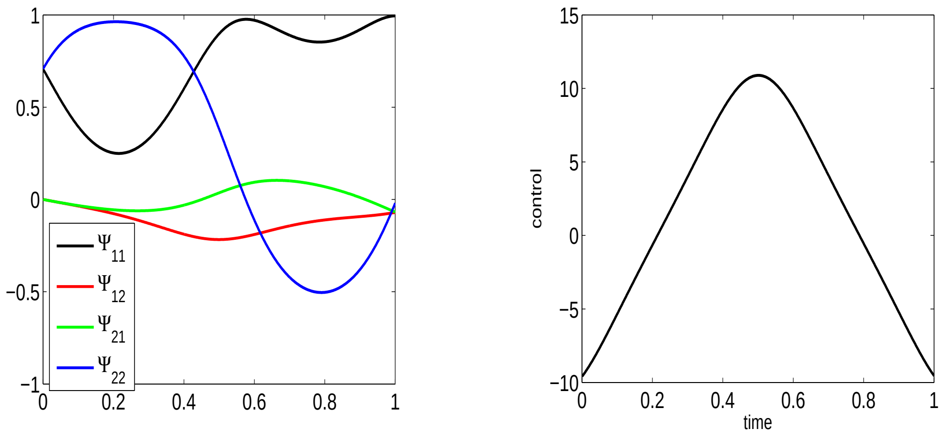

Figure 6.13: The trajectory and control from the state $|\Psi\rangle = \frac{1}{\sqrt{2}}[1, i]^T$ to the ground state $|g\rangle$ on a fixed time horizon $T = 1$ for the minimum norm problem

The necessary optimality system for the time optimal problem becomes

$$\frac{dx(t)}{dt} = \tau(Ax(t) + u(t)Bx(t)) \tag{6.74}$$

$$-\frac{dp(t)}{dt} = \tau(A + u(t)B)^T p(t) \tag{6.75}$$

$$u(t) = -\gamma \text{sign}(p(t)^T Bx(t)) \tag{6.76}$$

$$1 + \tau p(1)^T (A + Bu(1))x(1) = 0 \tag{6.77}$$

$$p(1) = \mu\,\mathcal{O} \tag{6.78}$$

$$x(0) = x_0, (x(1), \mathcal{O}) = 1 - \delta. \tag{6.79}$$

for $t \in [0, 1]$ and $\mu > 0$. For the regularized problem, the control $u(t)$ is smoothed by $u_\epsilon(t)$. Then the semi-smooth Newton method is applied to solve the regularized optimality system, which is a two-point boundary value problem. We take the shooting parameter to be $z = [p(0), \mu, \tau]$. In the numerical simulation, we set $\delta = 0.005$, $\Psi(0) = \frac{1}{\sqrt{2}}[1, i]^T$. Table 6.8 shows the time optimal solution τ for different control input γ. It is observed that with smaller γ, longer time is expected to take in order to drive the quantum state from $\Psi(0)$ to the ground state. When γ is less than 7, there are 2 switchings in the control in the form of $-1 \to 1 \to -1$. Figure 6.14 and Figure 6.15 show the trajectories and controls for cases $\gamma = 11$ and $\gamma = 7$.

Table 6.8: Time optimal solution with different γ for spin-$\frac{1}{2}$ system from $|\Psi\rangle = \frac{1}{\sqrt{2}}[1, i]^T$ to the ground state $|g\rangle = [1, 0]^T$.

γ	minimum τ	number of switch	control form
19.25	0.7236	0	1
11	1.0098	0	-1
8	1.3529	0	-1
7	1.1139	2	-1,1,-1
5	1.6516	2	-1,1,-1
3	2.8334	2	-1,1,-1
1	7.0563	2	-1,1,-1

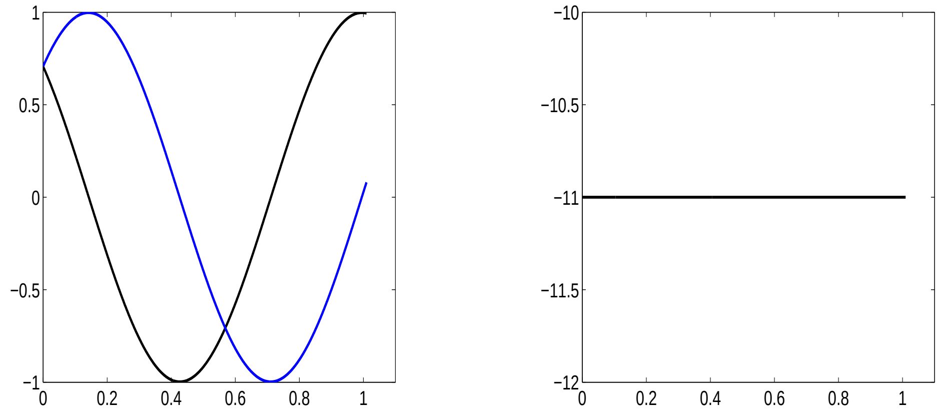

Figure 6.14: The Ψ_{11}, Ψ_{22} trajectory and control with $\gamma = 11$, the time optimal solution $\tau = 1.0098$

6.8 Control on Parabolic System

In this section, we consider the boundary control problem of parabolic PDE system governed by the following heat equation,

$$\frac{\partial y}{\partial t} = div(\kappa(x)\nabla y) \quad \text{in } [0, T] \times \Omega \tag{6.80}$$

$$y(0) = y_0, \tag{6.81}$$

$$\frac{\partial y}{\partial \nu} = v(t, x) \quad \forall x \in \partial\Omega = \Gamma \tag{6.82}$$

where y is the temperature distribution, $\kappa(x)$ is the heat conductivity, and ν is the outer normal on the boundary. The physical interpretation is as follows. Suppose in a thermal treatment of a body Ω within a chamber, we want to maintain the temperature within the

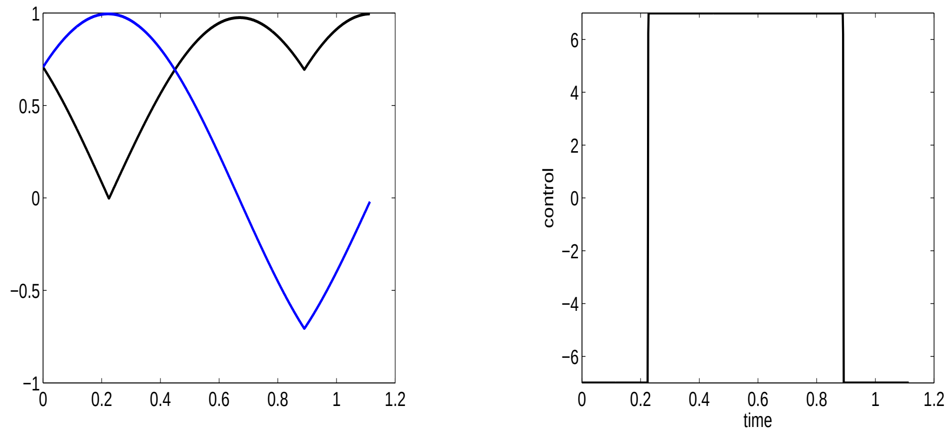

Figure 6.15: The Ψ_{11}, Ψ_{22} trajectory and control with $\gamma = 7$, the time optimal solution $\tau = 1.1139$

body at some equilibrium temperature $\bar{y}(t,x)$ by choosing a suitable boundary value v so that the temperature $y(t,x)$ is close to $\bar{y}(t;x)$ in Ω. (6.80)-(6.82) is known as flux boundary control problem for heat equation. The function $v(t,x)$ is the control input and $y(t,x)$ is the state variable, which belong to the control space $U = L^2(\Gamma)$ and the state space $X = H^1(\Omega)$ respectively.

We specify the control input by

$$v(t,x) = \sum_{i=1}^{n} b_i(x)u_i(t) \tag{6.83}$$

where $b_i(x) \in L^2(\Gamma)$ is the control distribution function, and $u_i(t)$ is the time dependent control input.

Our problem of interest is to find the flux boundary value $v(t,x)$ on the boundary Γ such that the temperature $y(t,x)$ is maintained at an equilibrium setting $y = 0$. For instance,

$$|y(T)|_{L^2} = \delta \tag{6.84}$$

for small $\delta > 0$. There can be different performance criterions for the control system. In particular, we consider the time optimal criterion and minimum effort criterion. Assume that there are control constraints, that is, $|u_i(t)| \le \gamma_i$, for $i = 1 \ldots n$. The cost functional to be minimized for time optimal control problem is to minimize running time T. The cost functional to be minimized for minimum effort control problem is to minimize $\frac{1}{2}\sum_{i=1}^{n}\gamma_i$.

For the ease of presentation, we present the one dimensional version of the boundary control of heat equation,

$$\frac{\partial y}{\partial t} = \Delta y \quad \text{in } [0,T]\times[0,1] \tag{6.85}$$

$$y(0,x) = y_0(x), \tag{6.86}$$

$$\frac{\partial}{\partial x} y(t,1) = u(t) \tag{6.87}$$

where $\kappa(x) = 1$, the physical domain $\Omega = [0,1]$, the control input $u(t) \in L^2(0,T)$ and the state variable $y(t) \in H^1(0,1)$.

Followed by [72], we write the boundary value problem (6.85)-(6.87) as a linear control system of the form (6.38) in a finite dimensional setting by a compact fourth order method discretization,

$$Q\frac{dy(t)}{dt} = -Hy + Bu(t), \quad y(0) = y_0 \tag{6.88}$$

where Q and H are $m\times m$ symmetric matrix, B is a m-dimensional vector in form of

$$Q = \begin{pmatrix} \frac{10}{12} & \frac{1}{12} & & \\ \frac{1}{12} & \frac{10}{12} & \ddots & \\ & \ddots & \ddots & \frac{1}{12} \\ & & \frac{1}{12} & \frac{10}{24} \end{pmatrix}_{m\times m} ; \quad H = m^2 \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & \ddots & \\ & \ddots & \ddots & -1 \\ & & -1 & 2 \end{pmatrix}_{m\times m} ; \quad B = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ m \end{pmatrix}_{m\times 1}.$$

here m is the number of nodes of discretization on $\Omega = [0,1]$.

The semi-discretization of time optimal control of heat equation can be formulated as follows:

$$\min \quad \tau \tag{6.89}$$

subject to

$$Q\frac{dy(t)}{dt} = -Hy + Bu(t), \quad y(0) = y_0 \tag{6.90}$$

$$|y(\tau)|_{L^2} = \delta, \tag{6.91}$$

$$|u(t)| \le \gamma, \quad t \in [0,\tau] \tag{6.92}$$

The necessary optimality system for the time optimal control problem (6.89)-(6.92) can be

Table 6.9: Time optimal solution for boundary control on heat equation with different control constraint γ

γ	δ	minimum time τ	number of switch
20	0.025	0.0888	5
10	0.025	0.1102	4
6	0.025	0.1331	4
4	0.025	0.1575	4
1	0.025	0.3126	3
1	0.05	0.2793	2

derived as

$$\begin{aligned}
&Q\frac{dy}{dt} = \tau(-Hy + Bu), \quad t \in [0,1] \\
&-Q\frac{dp}{dt} = -\tau\, H\, p \\
&u(t) = -\gamma\, \mathrm{sign}(B^T p) \\
&p(1) = \mu y(1) \\
&1 + \tau p^T(1)(-Hy(1) + Bu(1)) = 0, \\
&\frac{1}{2}(|y(1)|^2_{L^2} - \delta^2) = 0
\end{aligned}$$

For the regularized problem, the control $u(t)$ is smoothed by $u_\epsilon(t)$. Then the semismooth Newton method is applied to solve the regularized optimality system, which is a two-point boundary value problem. We take the shooting parameter to be $z = [p(0), \mu, \tau]$.

In the numerical simulation, $\Omega = (0,1)$ is uniformly discretized with $m = 10$, time step is set to be $\Delta t = 10^{-3}/4$ for time integration using Crank-Nicolson scheme. The initial temperature y_0 is set to be $y_0 = [\frac{1}{m}, \frac{2}{m}, \ldots, 1]^T$. Table 6.9 presents some time optimal solution for boundary control on heat equation with different control constraint γ. It is observed that larger control magnitude γ generates smaller minimum time τ and more switchings in the control input. The parameter δ measures how close the solution $y(T)$ to 0. It is observed that it requires less time to reach the target for smaller δ. Figure 6.16 shows the terminal state $y(T)$ and control for $\gamma = 10$.

Now we study the minimum effort control problem on heat equation. The cost functional to be minimized is

$$\min \quad \frac{1}{2}\gamma^2$$

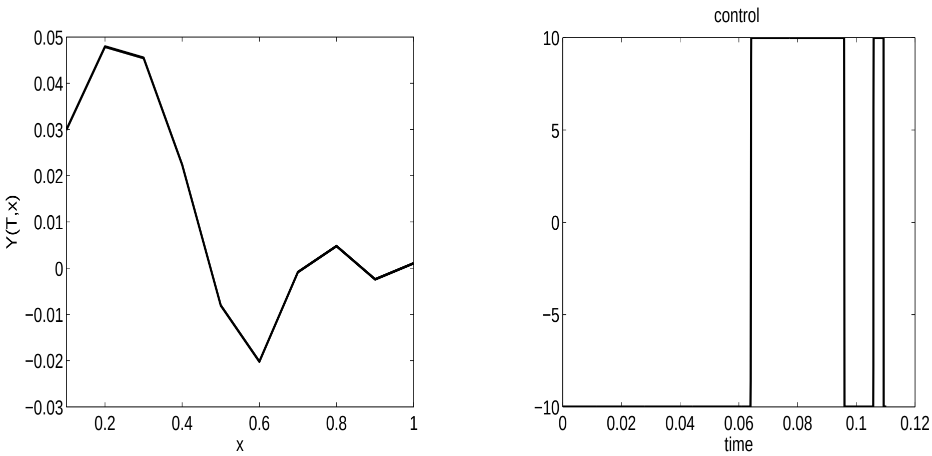

Figure 6.16: The terminal state and control of heat equation with $\gamma = 10$, the minimum time is $\tau = 0.1102$

subject to (6.90)-(6.92). The necessary optimality for minimum effort control is

$$
\begin{aligned}
&Q\frac{dy}{dt} = -Hy + Bu, \quad t \in [0, T] \\
&-Q\frac{dp}{dt} = -H\,p \\
&u(t) = -\gamma\,\mathrm{sign}(B^T p) \\
&p(T) = \mu y(T) \\
&\frac{1}{2}(|y(T)|^2_{L^2} - \delta^2) = 0 \\
&\gamma - \int_0^T |B^T p| dt = 0
\end{aligned}
$$

Table 6.10 presents some minimum effort solutions for boundary control on heat equation with different time horizon T. It is observed that it requires larger control magnitude γ if smaller time horizon is given or if smaller δ is given. Figure 6.17 shows the terminal state, control and state comparison with the uncontrolled state at time horizon $T = 0.1$. It is observed that, by applying the boundary control $u(t)$, the temperature $y(T)$ at time T gets much closer to the equilibrium $y = 0$ than the uncontrolled one. This means the boundary control technique is very effective. Figure 6.18 shows the control comparison with different δ for a fixed time horizon $T = 0.1$. The control pattern is observed to move to the left and magnitude becomes larger when δ becomes smaller.

Table 6.10: Minimum effort solution for boundary control on heat equation with different time horizon

time horizon τ	δ	exact γ	number of switch
0.5	0.05	0.4711	0
0.4	0.05	0.4928	1
0.3	0.05	0.8730	2
0.2	0.05	1.8924	3
0.1	0.05	9.1700	4
0.1	0.025	13.4338	4

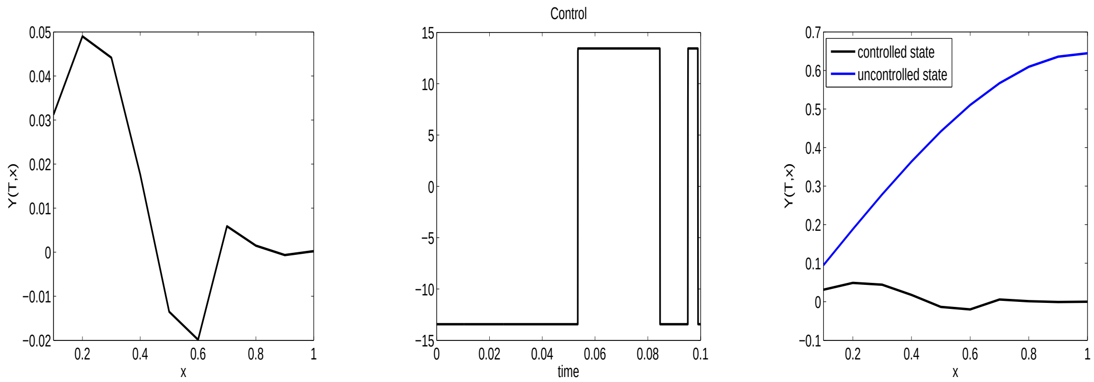

Figure 6.17: The terminal state, control and state comparison with the uncontrolled state at time horizon $T = 0.1$, minimum effort $\gamma = 13.4338$

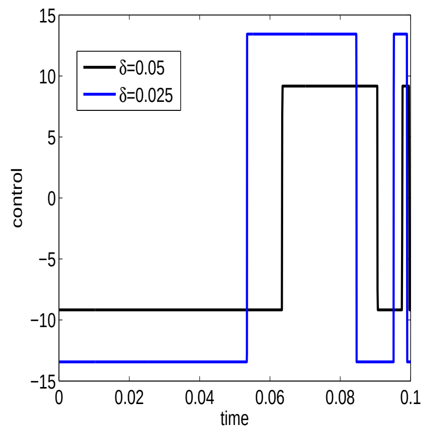

Figure 6.18: The control comparison with different δ for a fixed time horizon $T = 0.1$

Chapter 7

Conclusions and Future Work

7.1 Conclusions

In the thesis, we study the optimal control problem for bilinear systems, which arise in quantum control theory and tumor growth model. Specifically, we investigate and solve the problems of quantum feedback control, control of tumor growth dynamics and time optimal control for bilinear systems.

Quantum control theory has become an active research area from 1980s. In Chapter 2 and Chapter 3, optimal bilinear control for quantum system described by the Schrödinger equation is studied. The objective is to design a control law to drive the quantum state to an desired stable state. Based on the Lyapunov technique, we develop a nonlinear feedback synthesis with switching term to achieve the orbit tracking for the quantum systems. We implement the feedback law through a stable and accurate numerical method. Through numerical evidence, the tracking performance of our nonlinear feedback law significantly exceeds the performance of other existing feedback law. To further improve the orbit tracking performance of our proposed feedback law, we apply the receding horizon synthesis. Necessary optimality system for the optimal control problems on each short horizon is derived. Then we combine the second order accurate numerical integrations via time-splitting and the monotone convergent iterative scheme to solve the optimality system.

Quantum measurement is essential to be used to estimate the state of quantum systems. Followed by the quantum filtering theory, a quantum state subject to continuous measurement can be modeled by a classical stochastic differential equation, called quantum filtering equation. We study the problem of global stabilization of a quantum spin system under the noisy environment and continuous measurement via feedback control in Chapter 5. We design a new nonlinear control law with switching term to globally stabilize the quantum spin system at any arbitrary equilibrium state. We also develop and prove a positive definite preserving scheme for the time integration used in numerical simulations.

The switching mechanism in the feedback law developed for quantum control problem can be applied to a wide general class of control systems and feedback synthesis based on the Lyapunov stability. Hence we study the control problem of tumor growth, aiming at the reduction of the tumor cells population. We formulate the control problem based on existing mathematical models for tumor growth and develop the feedback law. Numerical evidence is shown to demonstrate the effectiveness of feedback law with switching term to suppress the tumor growth in Chapter 4.

Finally, we study the time optimal and minimum effort control problems for linear and bilinear systems in Chapter 6. To overcome the difficulties of nondifferentiability in the bang-bang control, a regularized problem is formulated and the semi-smooth Newton method is applied to solve the regularized optimality system. Our method is easy to implement and do not require accurate information on the switching structure in advance comparing to the existing shooting method. A lot of examples are studied to demonstrate the effectiveness of our method. In particular, we formulate the time optimal control problem for quantum spin-$\frac{1}{2}$ system and show the time optimal solution to a ground state. We also present the numerical results of time optimal control problem for infinite dimensional system through an example of heat equation by boundary control.

7.2 Future Work

Here are some projects we plan to work in the future.

- As shown in Theorem 2.6.1 and Lemma 2.6.1, in order to have asymptotic tracking properties by the proposed feedback law (2.22), the gap condition in the spectrum of internal Hamiltonian H_0 need to be satisfied. If it is not satisfied, we need to have multiple control inputs for our feedback law to work, which is demonstrated by the example of the harmonic oscillator. Hence our future work will include developing another control law which works with only one control input for the degenerate cases, for example, harmonic oscillator, in order to have asymptotic tracking properties.

- We believe the switching mechanism of the nonlinear feedback law (2.22) can be applied to other control problems to achieve better performance than the standard feedback law. We have succeeded in applying the methodology to the control problem of tumor growth model to achieve better performance. We would like to apply the feedback law to some other interesting control systems and models.

- We have applied the semi-smooth Newton method to solve time optimal and minimum effort control problem iteratively. An important issue is how to adjust the damping factor α adaptively to have global convergence of the numerical method. We are working on applying the Amijo-rule or Levenberg-Marquardt Method to achieve the global convergence of the Newton method.

- We also plan to work on another problem which is a mixture between the time optimal and minimum effort control problem. For example, the cost functional to be minimized is given by

$$\min \quad c\tau + (1-c)\gamma$$

  where $c \in [0, 1]$ is the mixture parameter. This problem is practically interesting since in reality we always want to have a good balance between effort and efficiency.

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