

論文 / 著書情報
Article / Book Information

題目(和文)	最速量子操作
Title(English)	Quantum brachistochrone
著者(和文)	奥平陽介
Author(English)	YOSUKE OKUDAIRA
出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第7080号, 授与年月日:2008年3月26日, 学位の種別:課程博士, 審査員:細谷 暁夫,白水 徹也
Citation(English)	Degree:Doctor of Science, Conferring organization: Tokyo Institute of Technology, Report number:甲第7080号, Conferred date:2008/3/26, Degree Type:Course doctor, Examiner;
学位種別(和文)	博士論文
Type(English)	Doctoral Thesis

— Thesis —

Quantum Brachistochrone

OKUDAIRA Yosuke

Department of Physics,
Tokyo Institute of Technology

February 2008

Abstract

We present a general framework for finding the time-optimal quantum evolution inspired by the classical problem called the brachistochrone problem. At first, the time-optimal control problem for achieving a pure state evolution from a given initial state to a desired final state is formulated. We minimize the duration time for this transition by finding the optimal control for the Hamiltonian in an available set subject to a certain constraint dictated by physical conditions. Then, it will be extended to the unitary evolution which has greater relevance for quantum computation. This provides a systematic way to make an efficient unitary gate on a certain physical system. To demonstrate this framework, we choose the anisotropic Heisenberg model and find a general solution. Since it is not always possible to find a general solution for the fundamental equation for the time-optimal control, we introduce the simulated annealing method as a simple numerical method to show that our framework can be used for the system whose general solution cannot be found. The numerical analysis based on the Krotov iteration method is introduced and applied to the time-optimal quantum control problem to solve the problem efficiently. The optimal realization of the quantum Fourier transform for two or more qubit systems are derived. We consider two generalizations of the quantum brachistochrone for mixed state evolutions. One is the unitary evolution with ancilla system ended up with the final measurement on the ancilla. The other is the repetition of measurement or decoherence model which can be represented by the evolution with the master equation in the Lindblad form. Also, the relation between the fidelity to the target and the duration time is considered.

Contents

1	Introduction	4
2	Preliminaries	7
2.1	Notations	7
2.2	Notation for the quantum circuit	8
3	Quantum brachistochrone	10
3.1	Brachistochrone problem	10
3.2	Quantum brachistochrone for pure states	11
3.3	Another way to formulate the quantum brachistochrone	14
3.4	Quantum brachistochrone for unitary operations	15
4	Applications	16
4.1	A simple example	16
4.2	One qubit model	18
4.3	Anisotropic Heisenberg model	21
4.3.1	Swap gate	24
4.3.2	Swap-like gate	27
4.3.3	Entangler gate	30
4.4	Dynamical or static	32
4.5	Discussion	33
4.6	Summary	34
5	Simulated annealing method	36
5.1	Interacting two 1/2 spins	37
5.1.1	Quantum brachistochrone equation	38
5.1.2	Result of the numerical computation	39
5.2	Superconducting flux qubits	41

5.2.1	Equations	41
5.2.2	Numerical analysis	42
5.3	Summary	43
6	The Krotov method	44
6.1	Formalism	44
6.2	Numerical procedure	45
6.3	Application to the unitary evolution	46
6.3.1	Convergence of the iterative method	46
6.3.2	Accuracy	49
6.4	Application to the time-optimal control	50
6.4.1	Fidelity optimal control	51
6.4.2	Low cost control	52
6.4.3	Constraints	53
6.4.4	Output recycling	54
6.5	Comparison with the analytic solution	54
6.6	Comparison with the simulated annealing method	55
6.7	Comparison with the conventional method	58
6.8	Example: quantum Fourier transform	59
6.9	Time evolution of the entanglement	62
6.10	Summary	62
7	Ancilla assisted quantum evolution	64
7.1	Two qubit model	64
8	Quantum brachistochrone for mixed states	67
8.1	Master equation	67
8.2	Invariance of the master equation	69
8.3	Optimal control problem	69
8.4	A one-qubit example	71
8.5	A model for open system	76
9	Summary and discussion	79
A	Quantum speed limit	83
A.1	Fubini-Study metric	83
A.2	Anandan-Aharonov bound	84
A.3	Margolus-Levitin bound	84

A.4 Quantum speed limit	85
B Nielsen’s geometric approach	86
C Quantum dots	88
D Construction of two-qubit gate with impulsive local operations	90
E Filtering technique	92
F Lower bound for QFT	94

Chapter 1

Introduction

The quantum mechanics discovered in the early 20th century is known to be a fundamental theory of physics. By the progress of technologies, quantum systems have gradually become manipulable in the late 20th century. Since Feynman suggested the quantum mechanical computers [1], it has been noticed that the computer based on quantum mechanics may be more efficient than the classical computer on some class of problems. Deutsch pioneered a fundamental concept of the quantum computation and quantum algorithms [2, 3]. By the discovery of Shor's factoring algorithm [4] and the Grover's search algorithm [5] the potential of quantum computation has been recognized and the effort to attain building blocks for that has been accelerated. The challenge of experimental realizations are directed on various candidate physical systems, e.g. nuclear spin, quantum dot, superconducting qubits or cavity QED. The quantum computation consists of unitary transformations and measurements. One obstacle for the realization is the effect of environment known as the decoherence which gradually reduces the coherence of the system by the uncontrollable interaction. In the coupled electron spins in semiconductor quantum dots [6], the coherence time for two-electron spin states exceeding 10^{-6} sec. has been observed. Recently, the superconducting qubits [7] have received a lot of attention, since the observed coherence times are improved from 10^{-9} sec. range to 10^{-6} sec. range [8].

There are several ways to reduce the effect of decoherence. The most promising method is the quantum error correction [9, 10, 11], which is to resort to redundancy in encoding information. In the Hilbert space of some physical systems, there is the decoherence-free subspace [12], which are decoupled from the environment. We may rely on making qubits in the decoherence-

free subspace. To avoid the decoherence and apply a unitary operation efficiently, it is important to steer the system in a time duration as short as possible.

In the quantum circuit model, it is known that any unitary operation can be decomposed into several elemental unitary operations for one or two qubits [13, 14]. Those elements are called the universal set of unitary operations or quantum gates [15]. Making those elements efficiently by the actual physical system is an important issue for realization of the quantum computation.

The speed of quantum gates is limited by the physical restriction on the state transition. The limits on the orthogonal time, which is required time to make a transition from a state to the orthogonal state, are derived by two independent considerations. Those derivations are briefly explained in Appendix A. But those considerations do not provide a framework for finding a time-optimal control.

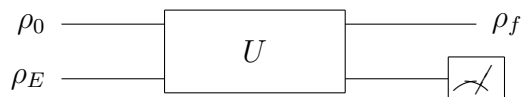
The optimal control theory for quantum systems is originally considered by Rabitz *et al.* [17]. Their theory provides a general framework for designing controls over molecular dynamics phenomena to maximize an expectation value, e.g. the occupation number of a state or the fidelity to a target wave packet. Recently, optimization problems for quantum systems get a lot of attentions in the context of quantum computation. Khaneja *et al.* [18] gave time-optimal control sequences for NMR experiments in which the one-qubit operation is assumed to be performed instantaneously. Zhang *et al.* [19] have shown a time-optimal realization of universal two-qubit gates in terms of the Cartan decomposition of Lie algebra generated by the set of available Hamiltonian. The conventional optimal control theory is defined for

$$i\frac{dU(t)}{dt} = \left(H_0 + \sum_{k=1}^m \varepsilon_k(t) H_k \right) U(t), \quad (1.1)$$

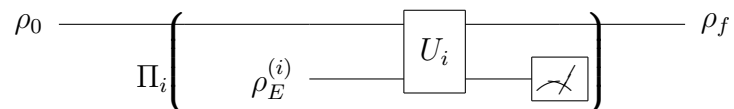
which is called *completely controllable* [27, 28] if any unitary operator U can be generated from identity operator. A necessary and sufficient condition for complete controllability is that the Lie algebra L_0 has dimension N^2 [21], where L_0 is generated by the available Hamiltonians $\{H_0, \dots, H_m\}$. The controllable parameters $\varepsilon_k(t)$ are frequently considered as unbounded functions.

So far, there is no effective and systematic way to find time-optimal controls which can be applied to any multi-qubit systems. In this thesis, we obtain the framework to find time-optimal controls for quantum systems based on the idea of the brachistochrone problem and demonstrate it. The system

and the available controls are represented by constraints for the Hamiltonian in the action in our framework. In Chapter 3, we firstly formulate the time optimization problem for the pure state evolution from a given initial state to a desired final state [22]. The extension for the unitary operations is straightforward. In Chapter 4 and 5, to exemplify our formulation, some models are solved analytically [23] and others are computed by the simulated annealing method. Chapter 6 is devoted to explain the Krotov iteration method and the way to apply it to the time-optimal quantum control problem. The demonstrations of this method for multi-qubit systems are also shown. Two extensions of the time-optimal control problem for mixed states are considered. The ancilla assisted system is considered in Chapter 7, which is an application of the time-optimal unitary operations formulated in Section 3.4. We consider the coherent composite system which has the ancilla system or the environment. The whole system evolves coherently and the environment is traced out at the end of the evolution.



In Chapter 8, we consider the repetition of measurements or decoherence which can be represented by the mixed state evolution governed by the master equation in the Lindblad form [24]. In the quantum circuit representation, this can be shown by



in which the component in the parenthesis is repeated with different $\rho_E^{(i)}$ and U_i . That is a natural extension of our framework for pure state evolution governed by the Schrödinger equation to the mixed states governed by the master equation.

Through this thesis, we consider the fidelity of the product on the way of time-optimal evolution toward the target as a function of time, since, in some cases, e.g. the quantum computation, it is necessary to estimate the trade-off between the fidelity and the time. Units are chosen such as $\hbar = 1$.

Chapter 2

Preliminaries

Before going into the contents, we introduce notations and conventions.

2.1 Notations

- N -dimensional Hilbert space: $\mathcal{H}_N$
- identity operator: I
- N -dimensional identity operator: I_N
- Pauli operators and the identity operator: $\sigma_x, \sigma_y, \sigma_z, \sigma_0$

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}, \quad \sigma_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (2.1)$$

- ladder operators: $\sigma_{\pm} = \frac{1}{2}(\sigma_x \pm i\sigma_y)$
- vector notation of Pauli operators: $\boldsymbol{\sigma} = (\sigma_x, \sigma_y, \sigma_z) = (\sigma_1, \sigma_2, \sigma_3)$
- inner product of $\boldsymbol{\sigma}$ and a vector $\mathbf{n} \in \mathbb{R}^3$: $\mathbf{n} \cdot \boldsymbol{\sigma} = \sum_i n_i \sigma_i$
- tensor product of identity operators and a Pauli operator in the i -th component: $\sigma_k^i = I \otimes \cdots \otimes \sigma_k \otimes \cdots \otimes I$
- qubit: The two-level quantum system which has eigenstates $|0\rangle$ and $|1\rangle$ (or $|\uparrow\rangle$ and $|\downarrow\rangle$) in $\mathcal{H}_2$.

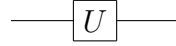
- binary representation of multi-qubits: (for 3 qubits as an example)

$$\begin{aligned}
|0\rangle &= |000\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \otimes |\uparrow\rangle \\
|1\rangle &= |001\rangle = |\uparrow\rangle \otimes |\uparrow\rangle \otimes |\downarrow\rangle \\
|2\rangle &= |010\rangle = |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\uparrow\rangle \\
|3\rangle &= |011\rangle = |\uparrow\rangle \otimes |\downarrow\rangle \otimes |\downarrow\rangle \\
|4\rangle &= |100\rangle = |\downarrow\rangle \otimes |\uparrow\rangle \otimes |\uparrow\rangle, \text{ and so on.}
\end{aligned}$$

- Hilbert-Schmidt inner product: $\langle A, B \rangle = \text{Tr}(A^\dagger B)$
- The Bloch sphere:
Any two-dimensional density operators can be represented as $\rho = \frac{1}{2}(I + \mathbf{x} \cdot \boldsymbol{\sigma})$ with the set $\{\mathbf{x} | \mathbf{x} \in \mathbb{R}^3, |\mathbf{x}| \leq 1\}$, which is called the Bloch sphere.

2.2 Notation for the quantum circuit

- unitary operation for a single qubit:



represents $U|\psi\rangle$ for $|\psi\rangle \in \mathcal{H}_2$. A single wire represents the state evolution of a single qubit from left to right.

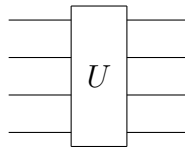
- Hadamard gate:

$$\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \text{---} \boxed{H} \text{---}$$

- Phase gate:

$$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\theta} \end{bmatrix} = \text{---} \boxed{\theta} \text{---}$$

- unitary operation for multiple qubit:



- swap gate:

$$U_{\text{swap}} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \begin{array}{c} \text{---} \times \text{---} \\ \text{---} \times \text{---} \end{array}$$

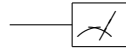
- controlled- U gate :

$$|0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes U = \begin{bmatrix} I & 0 \\ 0 & U \end{bmatrix} = \begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \boxed{U} \text{---} \end{array}$$

- controlled-NOT (CNOT) gate :

$$U_{\text{CNOT}} = |0\rangle\langle 0| \otimes I + |1\rangle\langle 1| \otimes \sigma_x = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{array}{c} \text{---} \bullet \text{---} \\ \text{---} \boxed{\sigma_x} \text{---} \end{array}$$

- measurement:



Chapter 3

Quantum brachistochrone

In this chapter, we formulate the time-optimal control to make a transition from a given initial state to a desired final state on a quantum system, which is based on the analogy in the classical mechanics. The system is assumed to be controllable by a set of available Hamiltonians dictated by the physical conditions. This framework is extended to the unitary operations regardless of the initial state.

3.1 Brachistochrone problem

Before going to the formulation of the optimal control problem on quantum mechanics, we recall an analogous problem in classical mechanics known as the brachistochrone problem. This problem was originally posed by Johann Bernoulli ¹ as a challenge to readers of the German scientific journal *Acta Eruditorum* in 1696 [16]. It was solved by Leibniz, L'Hospital, Newton and Jakob Bernoulli ² an elder brother of Johann, and the way invented by two Bernoullis was mathematically completed by Euler and Lagrange as the variational principle. The word “brachistochrone” is coming from the Greek words “βραχιστος” and “χρονος” which means “the shortest” and “time”, respectively.

In the brachistochrone problem one has to find the shape of a friction-free tube connecting two points and with a particle running inside subject only to homogeneous gravity. The solution, a segment of a cycloid, can be

¹also known as Jean or John (★1667 †1748)

²also known as James or Jacques (★1654 †1705).

found using the variational principle for the evolution time $T[\mathbf{x}(t)] = \int \frac{ds}{v}$, where the parameter s specifies the length of the tube from the initial to the current position $\mathbf{x}(t)$ of the particle, i.e. $ds^2 = |d\mathbf{x}|^2$. The magnitude of the particle's velocity is $v = \frac{ds}{dt} = \sqrt{2(E - V(\mathbf{x}))/m}$, where E is the conserved energy and V is the gravitational potential.

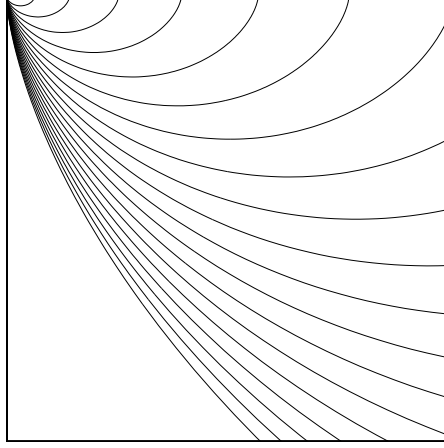


Figure 3.1: The curves derived by solving the brachistochrone problem. Those curves known as the cycloid are connecting any points below the x -axis and the origin at the left top.

3.2 Quantum brachistochrone for pure states

Let us formulate the quantum problem based on the idea of the classical brachistochrone problem. In the quantum case, the length of the tube is replaced by the distance between states. The duration time T for realizing some target state $|\psi_f\rangle$ is given by

$$T = \int_0^{s_f} \frac{dt}{ds} ds \quad (3.1)$$

where $|\psi(0)\rangle = |\psi_i\rangle$ and $|\psi(s_f)\rangle = |\psi_f\rangle$ and s is a parametrization of the curve. We will take the Fubini-Study metric for an infinitesimal length ds such that

$$ds^2 = \langle d\psi | (1 - |\psi\rangle\langle\psi|) | d\psi \rangle. \quad (3.2)$$

It gives velocity as the standard deviation of energy:

$$v = \frac{ds}{dt} \quad (3.3)$$

$$= \left(\left\langle \frac{d\psi}{dt} \middle| (1 - |\psi\rangle\langle\psi|) \middle| \frac{d\psi}{dt} \right\rangle \right)^{1/2} \quad (3.4)$$

$$= \left(\langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2 \right)^{1/2} \quad (3.5)$$

$$= \Delta E \quad (3.6)$$

where we have used the Schrödinger equation at (3.5). In this thesis, the Hamiltonian is considered to be traceless, since the trace part just drives the overall phase of the state which is irrelevant to the physics. We define the action as follows

$$S = \int \frac{ds}{v} + \int 2 \operatorname{Re} \langle \phi | (i \frac{d}{dt} - H) | \psi \rangle dt + \int \sum_m \lambda_m f_m(H) dp \quad (3.7)$$

where the first term gives the time duration [25], the second term ensures that the time evolution of pure state is governed by the Schrödinger equation and the last term consists of Lagrange multipliers λ_m and functions of the Hamiltonian impose constraints for the Hamiltonian

$$f_m(H) = 0. \quad (3.8)$$

To fix endpoints of the integral, we parametrize all terms with $p \in [0, 1]$ as follows

$$S = \int_0^1 dp \left[\frac{\frac{ds}{dp}}{v} + 2 \operatorname{Re} \langle \phi | \left(i \frac{d}{dp} - H \frac{\frac{ds}{dp}}{v} \right) | \psi \rangle + \sum_m \lambda_m f_m(H) \right] \quad (3.9)$$

$$= \int_0^1 dp \left[\left(1 - 2 \operatorname{Re} \langle \phi | H | \psi \rangle \right) \frac{\frac{ds}{dp}}{v} + 2 \operatorname{Re} \langle \phi | i \frac{d}{dp} | \psi \rangle + \sum_m \lambda_m f_m(H) \right] \quad (3.10)$$

where $|\psi(p=0)\rangle = |\psi_i\rangle$, $|\psi(p=1)\rangle = |\psi_f\rangle$ and

$$\frac{\frac{ds}{dp}}{v} = \frac{\sqrt{\langle \frac{d\psi}{dp} | (1 - |\psi\rangle\langle\psi|) | \frac{d\psi}{dp} \rangle}}{\Delta E}. \quad (3.11)$$

Taking the variation of S with respect to H , we have

$$\{G, |\psi\rangle\langle\psi|\} + |\psi\rangle\langle\phi| + |\phi\rangle\langle\psi| - F = 0 \quad (3.12)$$

where

$$F = \sum_m \lambda_m \frac{\partial f_m(H)}{\partial H} / \frac{dt}{dp} \quad (3.13)$$

$$G = (1 - 2 \operatorname{Re} \langle \psi | H | \phi \rangle) \frac{H - \langle H \rangle}{2(\Delta E)^2}. \quad (3.14)$$

Multiplying H and taking the trace, (3.12) gives

$$\operatorname{Tr} HF = 1. \quad (3.15)$$

Applying (3.12) to $|\psi\rangle$, we have

$$F = \{F, |\psi\rangle\langle\psi|\} - \langle F \rangle |\psi\rangle\langle\psi|. \quad (3.16)$$

The variation by $|\phi\rangle$ and $|\psi\rangle$ gives

$$i \frac{d}{dt} |\psi\rangle = H |\psi\rangle, \quad (3.17)$$

$$i \frac{d}{dt} |\phi\rangle + i \frac{dG}{dt} |\psi\rangle = H |\phi\rangle. \quad (3.18)$$

The variation with respect to the Lagrange multipliers λ_m gives the constraints $f_m(H) = 0$. Substituting (3.17) and (3.18) into the time derivative of (3.12), we obtain the fundamental equation what we call “quantum brachistochrone equation”

$$i \frac{d}{dt} F = [H, F]. \quad (3.19)$$

Once we have the constraint for the Hamiltonian, (3.13) gives the operator F which contains parameters of H . By solving (3.19) with a certain initial values $F(0)$ and $H(0)$ satisfying the condition (3.15) and (3.16), we obtain a time evolution of the Hamiltonian which gives the time-optimal evolution of $|\psi\rangle$ by integrating the Schrödinger equation. The desired transition for $|\psi_f\rangle$ can be found by choosing an appropriate initial condition $F(0)$ and $H(0)$.

3.3 Another way to formulate the quantum brachistochrone

In the previous section, we formulated the problem to find a time-optimal quantum evolution based on the idea of the classical brachistochrone problem. This section is devoted to show another view of the formulation for this problem. We introduce the action

$$S = \int_0^1 d\tau \left(\alpha + 2 \operatorname{Re}[\langle \phi | (i \frac{d}{d\tau} |\psi\rangle - \alpha H |\psi\rangle)] + \sum_m \lambda_m f_m(H) \right) \quad (3.20)$$

where the parameter τ is chosen so that $|\psi(0)\rangle = |\psi_i\rangle$ and $|\psi(1)\rangle = |\psi_f\rangle$. The first term gives the time duration and the second term ensures that the state evolution is governed by

$$i \frac{d}{d\tau} |\psi\rangle = \alpha H |\psi\rangle. \quad (3.21)$$

By choosing $dt = \alpha(t)d\tau$, (3.21) will be the Schrödinger equation

$$i \frac{d}{dt} |\psi\rangle = H |\psi\rangle. \quad (3.22)$$

The first term in the action is the physical time measured by the integral $\int_0^1 \alpha(\tau) d\tau$. The third term yields the constraints $f_m(H) = 0$ by taking variation with respect to the Lagrange multipliers λ_m . The variation with respect to α and H gives $2 \operatorname{Re}\langle \phi | H |\psi\rangle = 1$ and

$$|\phi\rangle\langle\psi| + |\psi\rangle\langle\phi| = F \quad (3.23)$$

where $F = \sum_m \lambda_m \frac{\partial f_m}{\partial H} / \alpha$. Taking variation with respect to $|\psi\rangle$, we obtain

$$i \frac{d}{d\tau} |\phi\rangle = \alpha H |\phi\rangle. \quad (3.24)$$

The time derivative of (3.23) with (3.21) and (3.24) reads the quantum brachistochrone equation $i\dot{F} = [H, F]$ again.

3.4 Quantum brachistochrone for unitary operations

For the purpose to generate the desired unitary operation for a quantum system regardless of the initial state, we formulate the time-optimal control problem for unitary operations. The action for time-optimal unitary operations is obtained by a small modification from (3.20)

$$S = \int_0^{\tau_1} d\tau \left(\alpha + 2 \operatorname{Re} \operatorname{Tr}[V^\dagger (i \frac{d}{d\tau} - \alpha H) U] + \sum_m \lambda_m f_m(H) \right) \quad (3.25)$$

where the parameter τ is chosen so that $U(0) = I$ and $U(\tau_1) = U_{\text{target}}$. The first term gives the time duration. By the variation with respect to V and U we have

$$i \frac{d}{d\tau} U = \alpha H U \quad (3.26)$$

$$i \frac{d}{d\tau} V = \alpha H V. \quad (3.27)$$

The Schrödinger equation in the physical time is given by the reparametrization $dt = \alpha(\tau)d\tau$. The variation with respect to α and H give $2 \operatorname{Re} \operatorname{Tr}(V^\dagger H U) = 1$ and

$$UV^\dagger + VU^\dagger = F \quad (3.28)$$

where $F = \sum_m \lambda_m \frac{\partial f_m}{\partial H} / \alpha$. The time derivative of (3.28) with (3.26) and (3.27) reads the quantum brachistochrone equation

$$i\dot{F} = [H, F] \quad (3.29)$$

again.

Once we have the constraints for the Hamiltonian $f_m(H)$, the operator F is obtained and (3.29) can be solved together with an initial condition $H(0)$ and Lagrange multipliers $\lambda_a(0)$ or $F(0)$. To obtain a particular optimal evolution which gives the target U_{target} , we have to find an appropriate initial condition. If we obtain the analytical solution of (3.29), we can fix some integration constants according to the target, namely the target determines the initial condition.

Chapter 4

Applications

To demonstrate this framework, we show some examples and corresponding solutions.

The unitary operation generated by a constant Hamiltonian H in a time duration Δt is

$$U = \exp[-iH\Delta t]. \quad (4.1)$$

It is easy to see that we can make the same unitary operation by the time $\Delta t/\alpha$ with Hamiltonian αH for any $\alpha \geq 0$. Thus, if there are no static components or boundaries for parameters in the Hamiltonian, we can make a transition arbitrarily fast by choosing large Hamiltonian. For those cases, we normalize the Hamiltonian

$$\text{Tr } H^2 = \text{constant}. \quad (4.2)$$

4.1 A simple example

To exemplify this method, we consider a simple constraint on the Hamiltonian

$$f(H) = \frac{1}{2}(\text{Tr } H^2 - 2\omega^2) = 0, \quad (4.3)$$

where ω is a positive constant. In this case, the operator F defined in (3.13) becomes

$$F = \mu H, \quad (4.4)$$

where $\mu = \lambda \frac{dt}{dp}$. The quantum brachistochrone equation (3.19) yields $H = \text{constant}$, since the relation (3.15) gives $\mu = \text{constant}$.

If we consider the time-optimal generation of unitary operations, the Hamiltonian is obtained by solving $e^{i\chi}U_{\text{target}} = \exp[-iHT]$, where χ is an arbitrary phase. It is always possible to diagonalize the target by a unitary W , i.e. $U_{\text{target}} = W \exp[-i\Lambda]W^\dagger$. By choosing χ which minimizes $\text{Tr}(\Lambda - \chi I)^2$, we obtain optimal Hamiltonian: $HT = W(\Lambda - \chi I)W^\dagger$ with the duration time T .

On the other hand, if we consider the time-optimal evolution of a pure state from $|\psi_i\rangle$ to $|\psi_f\rangle$, the equation (3.16) gives the relation between the Hamiltonian and the state

$$H = H|\psi\rangle\langle\psi| + |\psi\rangle\langle\psi|H \quad (4.5)$$

which gives $\langle H \rangle = 0$ and $\Delta E = \omega$. Using the Schrödinger equation, (4.5) can be seen as $H = i(|\dot{\psi}\rangle\langle\psi| - |\psi\rangle\langle\dot{\psi}|)$, whose time derivative is $0 = |\ddot{\psi}\rangle\langle\psi| - |\psi\rangle\langle\ddot{\psi}|$. Applying it to $|\psi\rangle$, we have $|\ddot{\psi}\rangle = -(\Delta E)^2|\psi\rangle$, which reads

$$|\psi(t)\rangle = \cos(\omega t)|\psi(0)\rangle + \frac{\sin(\omega t)}{\omega}|\dot{\psi}(0)\rangle. \quad (4.6)$$

We find the time-optimal evolution of the state from given initial state $|\psi_i\rangle$ to final state $|\psi_f\rangle$ as

$$|\psi(t)\rangle = \cos(\omega t)|\psi_i\rangle + \sin(\omega t)|\psi'_f\rangle, \quad (4.7)$$

where $|\psi'_f\rangle$ is normalized state of $|\psi_f\rangle - \langle\psi_i|\psi_f\rangle|\psi_i\rangle$. The optimal Hamiltonian is

$$H = i\omega(|\psi'_f\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi'_f|) \quad (4.8)$$

The optimal time to get $|\psi_f\rangle$ from $|\psi_i\rangle$ is

$$T = \frac{1}{\omega} \cos^{-1} |\langle\psi_i|\psi_f\rangle|. \quad (4.9)$$

The trajectory of the state (4.7) is along the equator of the Bloch sphere, which represent the projective space spanned by $|\psi_i\rangle$ and $|\psi'_f\rangle$ (see Figure 4.1 in which the coordinate is chosen so that two states on the Bloch sphere are on the xy -plane). The optimal time to make a transition between $\rho_i = \frac{1}{2}(I + \sigma)$ and $\rho_f = \frac{1}{2}(I + \cos\varphi\sigma_x + \sin\varphi\sigma_y)$ on the equator is $T = \frac{\varphi}{2\omega}$. If the initial and final states are orthogonal, the duration time coincides with the orthogonal time $t_\perp = \frac{\pi}{2\omega}$ obtained in appendixes A.2 and A.3, since $\Delta E = \omega$ and

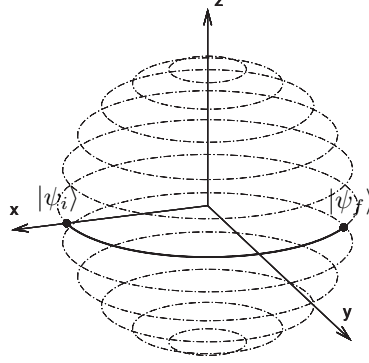


Figure 4.1: An optimal curve on the Bloch sphere. Any two points on the sphere are connected by the great circle. The direction of the magnetic field is along the z -axis in this figure. The dotted curves visualizes the Bloch sphere which represents the projective space spanned by the initial state and the final state.

$\langle E \rangle - E_0 = \omega$ where the expectation value of energy $\langle E \rangle = 0$ and the energy of the ground state $E_0 = -\omega$.

If the system is one qubit, the Hamiltonian can be taken as

$$H = \mathbf{B}(t) \cdot \boldsymbol{\sigma} \quad (4.10)$$

which is physically equivalent to the system of the $\frac{1}{2}$ -spin in the magnetic field $\mathbf{B}$. The trajectory of the state (4.7) on the Bloch sphere can be seen as a segment of a great circle on the sphere, and the magnetic field (4.8) is orthogonal to this circle.

4.2 One qubit model

As an example of this general framework we may consider the following case of one qubit subject to the two constraints

$$f_1(H) = \frac{1}{2}(\text{Tr } H^2 - 2\omega^2) = 0, \quad (4.11)$$

$$f_2(H) = \text{Tr}(H\sigma_z) = 0, \quad (4.12)$$

where σ_j ($j = x, y, z$) are the Pauli matrices. This corresponds to the physical situation where one can apply a magnetic field with x and y components only,

i.e. the available Hamiltonian is

$$H = B_x \sigma_x + B_y \sigma_y, \quad (4.13)$$

with the constraint $B_x^2 + B_y^2 = \omega^2$. Solving equations given from (3.29), we obtain

$$\begin{aligned} B_x(t) &= -\omega \sin 2(\Omega t + \varphi) \\ B_y(t) &= -\omega \cos 2(\Omega t + \varphi) \end{aligned} \quad (4.14)$$

where $\Omega = \lambda_2/\lambda_1$ is a constant and φ is an initial phase. The Baker-Campbell-Hausdorff formula leads to

$$H(t) = e^{i\Omega t \sigma_z} H(0) e^{-i\Omega t \sigma_z}. \quad (4.15)$$

The corresponding unitary matrix satisfies $i\dot{U} = e^{i\Omega t \sigma_z} H(0) e^{-i\Omega t \sigma_z} U$, whose solution is

$$U(t) = e^{i\Omega t \sigma_z} e^{-i(H(0) + \Omega \sigma_z)t}, \quad (4.16)$$

which can also be regarded as a time-optimal unitary operation.

Let us consider the case in which the initial state is on the equator of the Bloch sphere $\mathbb{C}P^1$, $\langle \sigma_z \rangle = 0$. Without loss of generality, we may choose $P(0) = (1 + \sigma_x)/2$, i.e. the spin initially points toward $(1, 0, 0)$. Then the condition $F(0) = \{F(0), P(0)\}$, which is characteristic of the time-optimal quantum evolution for pure states, and the constraints (4.11) and (4.12) imply that $H(0) = -\omega \sigma_y$ (and $\varphi = 0$), and from (4.15) and (4.16) we finally obtain

$$\langle \sigma \rangle(t) = \begin{bmatrix} \cos 2\Omega t \cos 2\Omega' t + \frac{\Omega}{\Omega'} \sin 2\Omega t \sin 2\Omega' t \\ -\sin 2\Omega t \cos 2\Omega' t + \frac{\Omega}{\Omega'} \cos 2\Omega t \sin 2\Omega' t \\ \frac{\omega}{\Omega'} \sin 2\Omega' t \end{bmatrix}$$

where $\Omega' = \sqrt{\omega^2 + \Omega^2}$. We can interpret $B_x(t)$ and $B_y(t)$ in (4.14) as a magnetic field rotating with angular velocity 2Ω . If the final state $|\psi_f\rangle$ is given, the angular velocity 2Ω and the time duration T are also determined. For instance, let us assume $P(T) = (1 + \cos \varphi \sigma_x + \sin \varphi \sigma_y)/2$, which is a point on the equator with longitude φ . The solution of angular velocity and optimal time is

$$\Omega = \frac{\omega(\varphi - \pi)}{\sqrt{2\pi\varphi - \varphi^2}}, \quad T = \frac{1}{2\omega} \sqrt{2\pi\varphi - \varphi^2}, \quad (4.17)$$

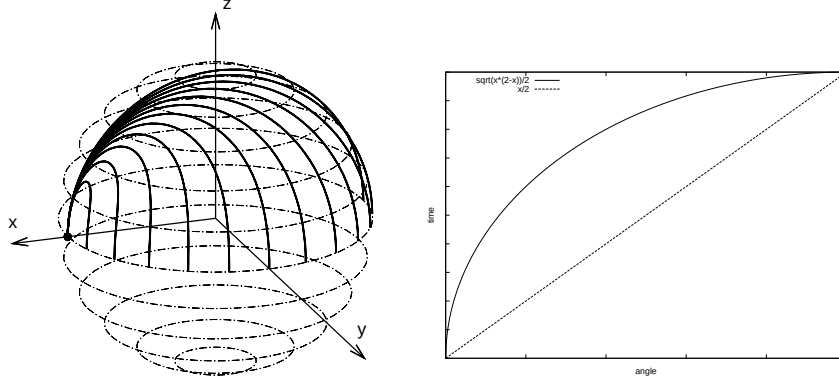


Figure 4.2: The left figure is a part of family of optimal curves on the Bloch sphere (solid curves). Antipodal points are connected by a great circle. The right figure is the comparison of duration times with the previous case for $\varphi \in [0, \pi]$. The solid curve is the optimal time required to make transition from $(1, 0, 0)$ to $(\cos \varphi, \sin \varphi, 0)$ on the Bloch sphere (4.17) and the dotted line is for the trajectory on the equator given in the previous section.

and corresponding trajectories are depicted in Figure 4.2. We can see that, every state represented by the point on the equator can be carried for arbitrary states on the Bloch sphere by the time-optimal Hamiltonian. Especially, the time-optimal path to the antipodal point is a great circle on the Bloch sphere and the duration time to realize this transition is $T = \frac{\pi}{2\omega}$, which is the same as the result of the previous section. From the left of Figure 4.2, it is obvious that the required time to make a transition from a point $(1, 0, 0)$ to another point $(\cos \varphi, \sin \varphi, 0)$ with $\varphi \in (0, \pi)$ given in this section is longer than that for the trajectory on the equator given in the previous section, due to the extra constraint (4.12).

4.3 Anisotropic Heisenberg model

Let us consider a couple of spins with the variable coupling strength and variable magnetic fields restricted to z -direction:

$$H = - \sum_k J_k(t) \sigma_k^1 \sigma_k^2 + B_1(t) \sigma_3^1 + B_2(t) \sigma_3^2 \quad (4.18)$$

where J_i are anisotropic coupling strength. In the matrix form, it can be seen

$$H = \begin{bmatrix} -J_3 + B_+ & 0 & 0 & -J_- \\ 0 & J_3 + B_- & -J_+ & 0 \\ 0 & -J_+ & J_3 - B_- & 0 \\ -J_- & 0 & 0 & -J_3 - B_+ \end{bmatrix} \quad (4.19)$$

where $B_{\pm} = B_1 \pm B_2$ and $J_{\pm} = J_1 \pm J_2$. We suppose that the remaining generators are prohibited, and impose the constraint on the Hamiltonian: $\text{Tr } H^2 = 4\omega^2$, i.e.

$$B_1^2 + B_2^2 + J_1^2 + J_2^2 + J_3^2 = \frac{1}{2}(B_+^2 + B_-^2 + J_+^2 + J_-^2) + J_3^2 = \omega^2 \quad (4.20)$$

where ω is a constant. These conditions are represented by following operator

$$F = \mu H + \sum_{ij} \lambda_{ij} \sigma_i^1 \sigma_j^2 + \xi_1 \sigma_1^1 + \xi_2 \sigma_1^2 + \eta_1 \sigma_2^1 + \eta_2 \sigma_2^2. \quad (4.21)$$

where $\lambda_{ii} = 0$. Once we get above operators, the first task is to solve the quantum brachistochrone equation $i\dot{F} = [H, F]$, to get the optimal Hamiltonian. In this case, μ is a constant since

$$0 = \text{Tr}(\dot{F}H) \quad (4.22)$$

$$= 4\dot{\mu}\omega^2. \quad (4.23)$$

Comparing coefficients of orthogonal generators in each side, we get 15 equations shown in the following list.

$$\mu \dot{B}_1 = 2(J_2 \lambda_{12} - J_1 \lambda_{21}) \quad (\text{from } \sigma_3^1) \quad (4.24)$$

$$\mu \dot{B}_2 = -2(J_1 \lambda_{12} - J_2 \lambda_{21}) \quad (\text{from } \sigma_3^2) \quad (4.25)$$

$$-\mu \dot{J}_1 = -2(B_1 \lambda_{21} + B_2 \lambda_{12}) \quad (\text{from } \sigma_1^1 \sigma_1^2) \quad (4.26)$$

$$-\mu \dot{J}_2 = 2(B_1 \lambda_{12} + B_2 \lambda_{21}) \quad (\text{from } \sigma_2^1 \sigma_2^2) \quad (4.27)$$

$$-\mu \dot{J}_3 = 0 \quad (\text{from } \sigma_3^1 \sigma_3^2) \quad (4.28)$$

$$\dot{\lambda}_{12} = 0 \quad (\text{from } \sigma_1^1 \sigma_2^2) \quad (4.29)$$

$$\dot{\lambda}_{21} = 0 \quad (\text{from } \sigma_2^1 \sigma_1^2) \quad (4.30)$$

$$\dot{\lambda}_{13} = 2(\eta_1 J_3 - \eta_2 J_1) - 2B_1 \lambda_{23} \quad (\text{from } \sigma_1^1 \sigma_3^2) \quad (4.31)$$

$$\dot{\lambda}_{31} = -2(\eta_1 J_1 - \eta_2 J_3) - 2B_2 \lambda_{32} \quad (\text{from } \sigma_3^1 \sigma_1^2) \quad (4.32)$$

$$\dot{\lambda}_{23} = -2(\xi_1 J_3 - \xi_2 J_2) + 2B_1 \lambda_{13} \quad (\text{from } \sigma_2^1 \sigma_3^2) \quad (4.33)$$

$$\dot{\lambda}_{32} = 2(\xi_1 J_2 - \xi_2 J_3) + 2B_2 \lambda_{31} \quad (\text{from } \sigma_3^1 \sigma_2^2) \quad (4.34)$$

$$\dot{\xi}_1 = 2(J_3 \lambda_{23} - J_2 \lambda_{32}) - 2B_1 \eta_1 \quad (\text{from } \sigma_1^1) \quad (4.35)$$

$$\dot{\xi}_2 = -2(J_2 \lambda_{23} - J_3 \lambda_{32}) - 2B_2 \eta_2 \quad (\text{from } \sigma_1^2) \quad (4.36)$$

$$\dot{\eta}_1 = 2(J_1 \lambda_{31} - J_3 \lambda_{13}) + 2B_1 \xi_1 \quad (\text{from } \sigma_2^2) \quad (4.37)$$

$$\dot{\eta}_2 = -2(J_3 \lambda_{31} - J_1 \lambda_{13}) + 2B_2 \xi_2 \quad (\text{from } \sigma_2^2) \quad (4.38)$$

Equations (4.28), (4.29) and (4.30) indicate that λ_{12} , λ_{21} and J_3 are constants. Equations from (4.31) through (4.38) are irrelevant to the control variables. Time derivatives of equations (4.24), (4.25), (4.26) and (4.27) yield

$$\dot{B}_\pm = \mp 2\gamma_\pm J_\mp \quad (4.39)$$

$$\dot{J}_\pm = \mp 2\gamma_\mp B_\mp \quad (4.40)$$

which can easily be solved as:

$$B_\pm(t) = B_{0\pm} \cos 2(\gamma_\pm t + \psi_\pm), \quad (4.41)$$

$$J_\pm(t) = \mp B_{0\mp} \sin 2(\gamma_\mp t + \psi_\mp), \quad (4.42)$$

where $B_{0\pm}, \psi_\pm, \gamma_\pm = (\lambda_{12} \pm \lambda_{21})/\mu$ are constants. Here, the Hamiltonian corresponding to an optimal control is given with 6 free parameters, which are amplitudes: J_3, B_+ and B_- with the constraint (4.20), frequencies of

oscillation: γ_+ and γ_- and initial phases ψ_+ and ψ_- . The constraint (4.20) now indicates

$$B_{0+}^2 + B_{0-}^2 + 2J_3^2 = 2\omega^2. \quad (4.43)$$

The remaining work is to integrate the Schrödinger equation $i\dot{U}(t) = H(t)U(t)$ to get the unitary matrix. It is easy to see each oscillating mode will not be mixed because the permutation $P = |00\rangle\langle 00| + |01\rangle\langle 10| + |10\rangle\langle 11| + |11\rangle\langle 01|$ makes the H block diagonal:

$$P^\dagger H P = \begin{bmatrix} H_+ & O \\ O & H_- \end{bmatrix}, \quad H_\pm = \begin{bmatrix} \mp J_3 + B_\pm & -J_\mp \\ -J_\mp & \mp J_3 - B_\pm \end{bmatrix}. \quad (4.44)$$

Substitute $B_\pm(t)$ and $J_\pm(t)$ by solutions (4.41) and (4.42) for $H_\pm$, and apply the Baker-Campbell-Hausdorff formula, $H_\pm$ become

$$H_\pm = e^{\pm i(\gamma_\pm t + \psi_\pm)\sigma_y} (\mp J_3 \sigma_0 + B_\pm \sigma_z) e^{\mp i(\gamma_\pm t + \psi_\pm)\sigma_y}. \quad (4.45)$$

The Schrödinger equation gives the time evolution of each block $i\dot{U}_\pm = H_\pm U_\pm$. On the rotating frame, $\tilde{U}_\pm = e^{-i(\gamma_\pm t + \psi_\pm)\sigma_y} U_\pm$ evolves by time independent Hamiltonians:

$$i\dot{\tilde{U}}_\pm = (\mp J_3 \sigma_0 + B_\pm \sigma_z \pm \gamma_\pm \sigma_y) \tilde{U}_\pm. \quad (4.46)$$

These solutions are

$$\tilde{U}_\pm(t) = e^{-i(\mp J_3 \sigma_0 + B_\pm \sigma_z \pm \gamma_\pm \sigma_y)t} \tilde{U}_\pm(0), \quad (4.47)$$

which can be seen, at the rest frame:

$$U_\pm(t) = e^{\pm i(\gamma_\pm t + \psi_\pm)\sigma_y} e^{-i(\mp J_3 \sigma_0 + B_\pm \sigma_z \pm \gamma_\pm \sigma_y)t} e^{\mp i\psi_\pm \sigma_y}, \quad (4.48)$$

when $U(0) = I$. Expanding exponents, it will be

$$U_\pm(t) = e^{\pm iJ_3 t} (\alpha_{0\pm}(t)\sigma_0 + i \sum_{k=x,y,z} \alpha_{k\pm}(t)\sigma_k) \quad (4.49)$$

whose coefficients of Pauli matrices are

$$\begin{aligned} \alpha_{0\pm}(t) &= \cos \gamma_\pm t \cos \Omega_\pm t + \frac{\gamma_\pm}{\Omega_\pm} \sin \gamma_\pm t \sin \Omega_\pm t, \\ \alpha_{x\pm}(t) &= \pm \frac{B_{0\pm}}{\Omega_\pm} \sin \Omega_\pm t \sin(\gamma_\pm t + 2\psi_\pm), \\ \alpha_{y\pm}(t) &= \pm (\sin \gamma_\pm t \cos \Omega_\pm t - \frac{\gamma_\pm}{\Omega_\pm} \cos \gamma_\pm t \sin \Omega_\pm t), \\ \alpha_{z\pm}(t) &= -\frac{B_{0\pm}}{\Omega_\pm} \sin \Omega_\pm t \cos(\gamma_\pm t + 2\psi_\pm), \end{aligned}$$

for (4.49) , where $\Omega_{\pm} = \sqrt{B_{0\pm}^2 + \gamma_{\pm}^2}$. More explicitly, we can see

$$U(t) = \begin{bmatrix} e^{iJ_3t}(\alpha_{0+} + i\alpha_{z+}) & 0 & 0 & e^{iJ_3t}(\alpha_{y+} + i\alpha_{x+}) \\ 0 & e^{-iJ_3t}(\alpha_{0-} + i\alpha_{z-}) & e^{-iJ_3t}(\alpha_{y-} + i\alpha_{x-}) & 0 \\ 0 & e^{-iJ_3t}(-\alpha_{y-} + i\alpha_{x-}) & e^{-iJ_3t}(\alpha_{0-} - i\alpha_{z-}) & 0 \\ e^{iJ_3t}(-\alpha_{y+} + i\alpha_{x+}) & 0 & 0 & e^{iJ_3t}(\alpha_{0+} - i\alpha_{z+}) \end{bmatrix}. \quad (4.50)$$

Note that there are unattainable unitary operations in this model, e.g. CNOT gate.

4.3.1 Swap gate

Let us assume the target to be the SWAP gate up to an arbitrary phase

$$U_{\text{SWAP}} = e^{i\chi} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (4.51)$$

which swaps states of the first qubit and the second qubit, $U_{\text{SWAP}}|\psi\rangle \otimes |\phi\rangle = |\phi\rangle \otimes |\psi\rangle$. As the final condition at $t = T$, components of unitary operator (4.50) must satisfy

$$\alpha_{x+} - i\alpha_{y+} = 0 \quad (4.52)$$

$$\text{and } \alpha_{0-} + \alpha_{z-} = 0. \quad (4.53)$$

Equality (4.52) requires at least one of following conditions

$$B_{0+} = 0, \quad (4.54)$$

$$\{\gamma_+ = 0 \text{ and } 2\psi_+ = \pi N_{\psi_+}\}, \quad (4.55)$$

$$\{\gamma_+T = \pi N_{\gamma_+} \text{ and } \Omega_+T = \pi N_{\Omega_+}\} \quad (4.56)$$

$$\text{or } \{\gamma_+T = \pi N_{\gamma_+} - 2\psi_+ \text{ and } \Omega_+T = \pi N_{\Omega_+} - \delta_+\} \quad (4.57)$$

where $\delta_+ = \tan^{-1}(\frac{\Omega_+}{\gamma_+} \tan 2\psi_+)$ and N_X indicates integer related to a parameter X henceforth. From (4.54) through (4.57), we have

$$(4.54) \rightarrow U_+ = e^{iJ_3T} I \quad (4.58)$$

$$(4.55) \rightarrow U_+ = e^{iJ_3T} \begin{bmatrix} e^{-i(-)^{N_{\psi_+} B_{0+}T}} & 0 \\ 0 & e^{i(-)^{N_{\psi_+} B_{0+}T}} \end{bmatrix} \quad (4.59)$$

$$(4.56) \rightarrow U_+ = e^{i(J_3T + \pi(N_{\gamma_+} + N_{\Omega_+}))} I \quad (4.60)$$

$$(4.57) \rightarrow U_+ = e^{i(J_3T + \pi(N_{\gamma_+} + N_{\Omega_+}))} \begin{bmatrix} e^{i\nu_+} & 0 \\ 0 & e^{-i\nu_+} \end{bmatrix}, \quad (4.61)$$

respectively, where $\nu_+ = \tan^{-1}(\frac{B_{0+}}{\gamma_+} \sin 2\psi_+)$. On the other hand, (4.53) requires at least one of

$$\{\gamma_- = 0, \quad B_{0-}T = \pi N_{B_{0-}} + \frac{\pi}{2} \quad \text{and} \quad 2\psi_- = \pi N_{\psi_-} + \frac{\pi}{2}\}, \quad (4.62)$$

$$\{\gamma_-T = \pi N_{\gamma_-} + \frac{\pi}{2} \quad \text{and} \quad \Omega_-T = \pi N_{\Omega_-}\} \quad (4.63)$$

$$\text{or } \{\gamma_-T = \pi N_{\gamma_-} + \frac{\pi}{2} - 2\psi_- \quad \text{and} \quad \Omega_-T = \pi N_{\Omega_-} - \delta_-\} \quad (4.64)$$

respectively, where $\delta_- = \tan^{-1}(\frac{\Omega_-}{\gamma_-} \tan 2\psi_-)$. From (4.62) through (4.64), we have

$$(4.62) \rightarrow U_- = e^{-i(J_3T + \frac{\pi}{2} - \pi(N_{B_{0-}} + N_{\psi_-}))} \sigma_x \quad (4.65)$$

$$(4.63) \rightarrow U_- = e^{-i(J_3T - \pi(N_{\gamma_-} + N_{\Omega_-}))} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \quad (4.66)$$

$$(4.64) \rightarrow U_- = e^{-i(J_3T - \pi(N_{\gamma_-} + N_{\Omega_-}))} \begin{bmatrix} 0 & -e^{i\nu_-} \\ e^{-i\nu_-} & 0 \end{bmatrix} \quad (4.67)$$

where $\nu_- = \tan^{-1}(\frac{B_{0-}}{\gamma_-} \sin 2\psi_-)$.

To make unitary transformation U_{SWAP} , the block $U_-(T)$ must be proportional to σ_x , which requires the condition (4.62):

$$B_{0-}T = \pi N_{B_{0-}} + \frac{\pi}{2} \quad (4.68)$$

$$\text{and } J_3T + \chi = -\frac{\pi}{2} + \pi(N_{B_{0-}} + N_{\psi_-}) + 2\pi N_{U_-} \quad (4.69)$$

and the block $U_+(T)$ must be proportional to I , which requires (4.54) or (4.56). If we choose the condition (4.54), which requires

$$J_3T - \chi = 2\pi N_{U_+}. \quad (4.70)$$

Solving two relations (4.69) and (4.70), we obtain

$$J_3 T = \pi \left\{ -\frac{1}{4} + \frac{1}{2}(N_{B_{0-}} + N_{\psi_-}) + N_{U_+} + N_{U_-} \right\} \quad (4.71)$$

$$\chi = \pi \left\{ -\frac{1}{4} + \frac{1}{2}(N_{B_{0-}} + N_{\psi_-}) + N_{U_+} - N_{U_-} \right\}. \quad (4.72)$$

Multiplying T to the constraint (4.43)¹, ωT can be seen in terms of (4.54), (4.68) and (4.71). There is a set of integers $\{N_X\}$ which yields minimum time T by

$$\left(\frac{\omega T}{\pi} \right)^2 = \min_{\{N_X\}} \left[\frac{1}{2}(N_{B_{0-}} + \frac{1}{2})^2 + \left\{ -\frac{1}{4} + \frac{1}{2}(N_{B_{0-}} + N_{\psi_-}) + N_{U_+} + N_{U_-} \right\}^2 \right], \quad (4.73)$$

which leads to the extremal time and the corresponding Hamiltonian:

$$\omega T = \frac{\sqrt{3}}{4}\pi, \quad H = (-)^s \frac{\omega}{\sqrt{3}} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (4.74)$$

where $s = N_{B_{0-}} + N_{\psi_-}$. This solution is obtained when one choose $N_{U_+} = N_{U_-} = 0$ and $(N_{B_{0-}}, s) = (-1, 0), (-1, 1), (0, 0)$ or $(0, 1)$.

If we choose the other condition (4.56), which requires

$$\gamma_+ T = \pi N_{\gamma_+} \quad (4.75)$$

$$\Omega_+ T = \pi N_{\Omega_+} \geq |\pi N_{\gamma_+}|, \quad (4.76)$$

where the inequality of the second line comes from $(B_{0+}T)^2 = (\Omega_+T)^2 - (\gamma_+T)^2 \geq 0$. From the phase factor of U_+ , we have

$$J_3 T - \chi = 2\pi N_{U_+} - \pi(N_{\gamma_+} + N_{\Omega_+}), \quad (4.77)$$

which gives

$$\begin{aligned} J_3 T &= \pi(N_{U_+} + N_{U_-}) + \frac{\pi}{2}(N_{B_{0-}} + N_{\psi_-} - N_{\gamma_+} - N_{\Omega_+}) - \frac{\pi}{4} \\ \chi &= \pi(N_{U_+} - N_{U_-}) + \frac{\pi}{2}(N_{B_{0-}} + N_{\psi_-} + N_{\gamma_+} + N_{\Omega_+}) - \frac{\pi}{4} \end{aligned}$$

by using the relation (4.69). The constraint (4.43) yields minimum time T by

$$\begin{aligned} 2 \left(\frac{\omega T}{\pi} \right)^2 &= \min_{\{N_X\}} \left[(N_{B_{0-}} + \frac{1}{2})^2 + (N_{\Omega_+}^2 - N_{\gamma_+}^2) \right. \\ &\quad \left. + 2 \left\{ (N_{U_+} + N_{U_-}) + \frac{1}{2}(N_{B_{0-}} + N_{\psi_-} - N_{\gamma_+} - N_{\Omega_+}) - \frac{1}{4} \right\}^2 \right], \quad (4.78) \end{aligned}$$

$$^1(\omega T)^2 = \left\{ \frac{1}{2}(B_{0+}T)^2 + \frac{1}{2}(B_{0-}T)^2 + (J_3 T)^2 \right\}^2$$

which ends up with $B_{0+} = 0$, the same as (4.54) considered above, when all integers are zero. Therefore, (4.74) is the set of minimum time and the corresponding Hamiltonian. The list of constants for this case is as follows,

$$\begin{aligned} B_{0+} &= 0, & B_{0-} &= \frac{2\omega}{\sqrt{3}}, & J_3 &= \frac{\omega}{\sqrt{3}}, \\ \gamma_+ &= \text{any}, & \gamma_- &= 0, \\ \psi_+ &= 0, & \psi_- &= \frac{3\pi}{4} \end{aligned} \quad (4.79)$$

Let us consider the time evolution of the fidelity between the time-optimal generation of the unitary operator and the target, in which we define the fidelity between two unitary matrices U_1 and U_2 as $f(U_1, U_2) = \frac{1}{4} |\text{Tr}(U_1^\dagger U_2)|$. The fidelity can be written as a function of the duration time;

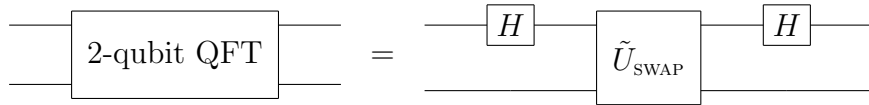
$$f(t) = \frac{1}{2} \sqrt{1 + 3 \sin^2 \frac{\pi t}{2T}}, \quad T = \frac{\sqrt{3}\pi}{4\omega}. \quad (4.80)$$

4.3.2 Swap-like gate

Let us consider to realize the swap-like gate $\tilde{U}_{\text{SWAP}}$ in optimal duration time up to phase:

$$\tilde{U}_{\text{SWAP}} = e^{i\chi} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & i \end{bmatrix}. \quad (4.81)$$

This gate can be a part of quantum Fourier transform.



The components of $U(T)$ in (4.50) must satisfy two conditions, what one is from (4.54) through (4.57) and the other is from (4.62) through (4.64), like as before. Since U_- must be proportional to σ_x , we require the condition (4.62):

$$B_{0-}T = \pi N_{B_{0-}} + \frac{\pi}{2} \quad (4.82)$$

$$J_3T + \chi = -\frac{\pi}{2} + \pi(N_{B_{0-}} + N_{\psi_-}) + 2\pi N_{U_-}. \quad (4.83)$$

The target requires (4.55) or (4.57), in which U_+ must be diagonal other than I . If we choose the condition (4.55), we have

$$J_3 T - \chi - (-)^{N_{\psi_+}} B_{0+} T = 2\pi N_{U_{+1}} \quad (4.84)$$

$$J_3 T - \chi + (-)^{N_{\psi_+}} B_{0+} T = 2\pi N_{U_{+2}} + \frac{\pi}{2}. \quad (4.85)$$

Solving a set of simultaneous equations (4.83), (4.84) and (4.85),

$$B_{0+} T = (-)^{N_{\psi_+}} \{-\pi(N_{U_{+1}} - N_{U_{+2}}) + \frac{\pi}{4}\} \quad (4.86)$$

$$J_3 T = \frac{\pi}{2}(2N_{U_-} + N_{U_{+1}} + N_{U_{+2}} + N_{B_{0-}} + N_{\psi_-}) - \frac{\pi}{8} \quad (4.87)$$

$$\chi = \frac{\pi}{2}(2N_{U_-} - N_{U_{+1}} - N_{U_{+2}} + N_{B_{0-}} + N_{\psi_-}) - \frac{3\pi}{8} \quad (4.88)$$

The minimum time T is given from the constraint (4.43) by substituting (4.82), (4.86) and (4.87),

$$2 \left(\frac{\omega T}{\pi} \right)^2 = \min_{\{N_X\}} [(N_{B_{0-}} + \frac{1}{2})^2 + (N_{U_{+1}} - N_{U_{+2}} - \frac{1}{4})^2 + 2\{\frac{1}{2}(2N_{U_-} + N_{U_{+1}} + N_{U_{+2}} + N_{B_{0-}} + N_{\psi_-} - \frac{1}{4})\}^2], \quad (4.89)$$

which gives a candidate of the minimum time and optimal Hamiltonian:

$$\omega T = \frac{\sqrt{11}}{8}\pi, \quad H = \frac{\omega}{\sqrt{11}} \begin{bmatrix} 3 & 0 & 0 & 0 \\ 0 & -1 & 4 & 0 \\ 0 & 4 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \quad (4.90)$$

when all integers are zero. The list of constants for this case is follows.

$$\begin{aligned} B_{0+} &= \frac{2\omega}{\sqrt{11}}, & B_{0-} &= \frac{4\omega}{\sqrt{11}}, \\ \gamma_+ &= 0, & \gamma_- &= 0, \\ \psi_+ &= 0, & \psi_- &= \frac{\pi}{4}, \\ J_z &= -\frac{\omega}{\sqrt{11}}. \end{aligned} \quad (4.91)$$

Whereas, if we choose the condition (4.57), we have

$$\begin{aligned} B_{0-} T &= \pi(N_{B_{0-}} + \frac{1}{2}) \\ J_3 T + \chi &= \pi(N_{B_{0-}} + N_{\psi_-}) + 2\pi N_{U_-} - \frac{\pi}{2} \\ J_3 T + \nu_+ - \chi &= -\pi(N_{\Omega_+} + N_{\gamma_+}) + 2\pi N_{U_{+1}} \\ J_3 T - \nu_+ - \chi &= -\pi(N_{\Omega_+} + N_{\gamma_+}) + 2\pi N_{U_{+2}} + \frac{\pi}{2} \end{aligned}$$

which gives

$$\begin{aligned} J_3 T &= \frac{\pi}{2}(2N_{U_-} + N_{U_{+1}} + N_{U_{+2}} - N_{\gamma_+} - N_{\Omega_+} + N_{B_{0-}} + N_{\psi_-} - \frac{1}{4}) \\ \chi &= \frac{\pi}{2}(2N_{U_-} - N_{U_{+1}} - N_{U_{+2}} + N_{\gamma_+} + N_{\Omega_+} + N_{B_{0-}} + N_{\psi_-} - \frac{3}{4}) \\ \nu_+ &= \pi(N_{U_{+1}} - N_{U_{+2}} - \frac{1}{4}). \end{aligned}$$

The constraint (4.43) leads to the minimum time

$$\begin{aligned} 2 \left(\frac{\omega T}{\pi} \right)^2 &= \min_{\{N_X\}, \psi_+, \delta_+} \left((N_{B_{0-}} + \frac{1}{2})^2 + \{ (N_{\Omega_+} - \frac{\delta_+}{\pi})^2 - (N_{\gamma_+} - \frac{2\psi_+}{\pi})^2 \} \right. \\ &\quad \left. + 2 \{ \frac{1}{2}(2N_{U_-} + N_{U_{+1}} + N_{U_{+2}} - N_{\gamma_+} - N_{\Omega_+} + N_{B_{0-}} + N_{\psi_-} + \frac{1}{4}) \}^2 \right) \end{aligned} \quad (4.92)$$

with conditions

$$1 = \sin^2 2\psi_+ \frac{(N_{\Omega_+} - \frac{\delta_+}{\pi})^2 - (N_{\gamma_+} - \frac{2\psi_+}{\pi})^2}{(N_{\gamma_+} - \frac{2\psi_+}{\pi})^2}, \quad (4.93)$$

$$\tan \delta_+ = \frac{N_{\Omega_+} - \frac{\delta_+}{\pi}}{N_{\gamma_+} - \frac{2\psi_+}{\pi}} \tan 2\psi_+ \quad (4.94)$$

where the minimization is taken with conditions (4.93), (4.94) and the second parenthesis of right hand side of (4.92) must be positive. Using (4.93) and reorganizing integers, (4.92) leads to

$$\begin{aligned} \left(\frac{\omega T}{\pi} \right)^2 &= \min_{m, n, x} \left[\frac{1}{2}(m + \frac{1}{2})^2 + \frac{x^2}{2\pi^2 \sin^2 x} + \frac{1}{4}(n + \frac{1}{4})^2 \right] \\ &\geq \left(\frac{3}{8} \right)^2 + \frac{1}{2\pi^2} > \left(\frac{\sqrt{11}}{8} \right)^2, \end{aligned}$$

since $\frac{x^2}{\sin^2 x} \geq 1$. Here, the lower bound is given regardless of (4.94). Whether or not there exist solutions for (4.92) with regarding (4.93) and (4.94), this condition, thus, can not achieve the optimal time shorter than previous case. Therefore, (4.90) is the set of the minimum time and the corresponding time-optimal Hamiltonian. The fidelity as a function of the duration time is given as follows

$$f(t) = \frac{1}{4} \sqrt{2 + 6 \sin \frac{\pi t}{2T} + 8 \sin^2 \frac{\pi t}{2T}}, \quad T = \frac{\sqrt{11}\pi}{8\omega}. \quad (4.95)$$

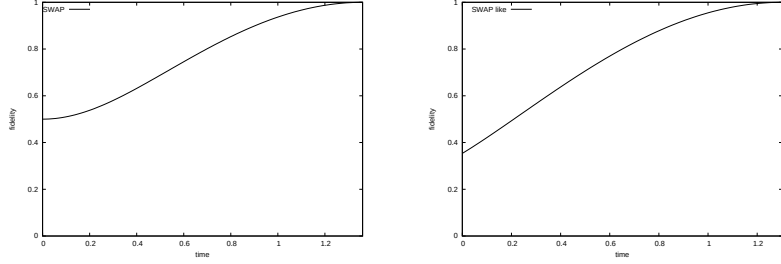


Figure 4.3: The time evolution of the fidelity $f(t) = \frac{1}{4} |\text{Tr } U(t)U_{\text{target}}^\dagger|$, where $U(t)$ is the time-optimal evolution to the target operator. The left figure is the evolution toward the swap gate and the right is toward the swap-like gate.

4.3.3 Entangler gate

As a last example, we want to find the optimal way to generate the entangler gate

$$U_{\text{ENT}} = e^{i\chi} \begin{bmatrix} \cos \varphi & 0 & 0 & \sin \varphi \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sin \varphi & 0 & 0 & \cos \varphi \end{bmatrix}, \quad (4.96)$$

where we choose the angle $\varphi \in [0, 2\pi]$. This gate, upon acting on the initial state $|00\rangle$, produces the φ -dependent entangled state $\cos \varphi |00\rangle - \sin \varphi |11\rangle$. For example, when $\varphi = \pm\pi/4 \pmod{2\pi}$, this allows reaching the maximally entangled Bell states $|\Phi^\pm\rangle = (|00\rangle \pm |11\rangle)/\sqrt{2}$. As usual, comparison of (4.50) and (4.96) gives the optimal time and Hamiltonian. The central block of U must satisfy

$$U_-(T) = e^{i\chi} I, \quad (4.97)$$

which leads to $\alpha_{x-} = \alpha_{y-} = \alpha_{z-} = 0$, thus we have

$$B_{0-} = 0 \quad \text{and} \quad \chi = -J_3 T + 2\pi N_-. \quad (4.98)$$

The rest requires

$$U_+(T) = e^{i\chi} \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix}, \quad (4.99)$$

which leads to $\Omega_+ T = \pi N_\Omega$ and

$$e^{i(J_3 T + \pi N_\Omega)} \begin{bmatrix} \cos \gamma_+ T & \sin \gamma_+ T \\ -\sin \gamma_+ T & \cos \gamma_+ T \end{bmatrix} = e^{i\chi} \begin{bmatrix} \cos \varphi & \sin \varphi \\ -\sin \varphi & \cos \varphi \end{bmatrix}, \quad (4.100)$$

in other words,

$$\chi = J_3 T + \pi N_\Omega + 2\pi N_+ \quad (4.101)$$

$$\gamma_+ T = \varphi + 2\pi N_\gamma. \quad (4.102)$$

Together with (4.98), we get

$$J_3 T = \pi(N_- - N_+ - \tfrac{1}{2}N_\Omega) \quad (4.103)$$

$$\chi = \pi(N_- + N_+ + \tfrac{1}{2}N_\Omega). \quad (4.104)$$

The constraint (4.43) gives the minimum time:

$$2 \left(\frac{\omega T}{\pi} \right)^2 = \min_{\{N_X\}} \left\{ N_\Omega^2 - \left(\frac{\varphi}{\pi} + 2N_\gamma \right)^2 + 2(N_- - N_+ - \tfrac{1}{2}N_\Omega)^2 \right\}. \quad (4.105)$$

It attains the minimum by choosing $N_\Omega = 2$, $N_- - N_+ = 1$ and $N_\gamma = -1$, the list of constants obtained for this target is given as

$$B_{0+} = \pm\sqrt{2}\omega, \quad B_{0-} = J_3 = 0, \quad \gamma_+ = \frac{\varphi - 2\pi}{T_{\text{ENT}}} \quad (4.106)$$

with the other constants being arbitrary. The optimal time and the corresponding Hamiltonian are

$$\omega T_{\text{ENT}}(\varphi) = \sqrt{\tfrac{1}{2}\varphi(2\pi - \varphi)}, \quad H(t) = \pm\sqrt{2}\omega \begin{bmatrix} -\cos \theta(t) & 0 & 0 & \sin \theta(t) \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \sin \theta(t) & 0 & 0 & \cos \theta(t) \end{bmatrix}, \quad (4.107)$$

where $\theta(t) = 2(\gamma_+ t + \psi_+)$. This case ends up with the dynamical Hamiltonian.

Note that, instead of (4.96), the entangler

$$U_{\text{ENT}} = e^{i\chi} \begin{bmatrix} \cos \varphi & 0 & 0 & -i \sin \varphi \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -i \sin \varphi & 0 & 0 & \cos \varphi \end{bmatrix}, \quad (4.108)$$

can be generated with the optimal time and the optimal Hamiltonian

$$\omega T_{\text{ENT}'}(\varphi) = \frac{\varphi}{\sqrt{2}}, \quad H = \sqrt{2}\omega \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad (4.109)$$

by choosing $B_{0+} = -\sqrt{2}\omega, B_{0-} = J_3 = 0, \gamma_+ = 0$ and $\cos 2\psi_+ = 0$. In particular, to make a maximally entangled state from $|00\rangle$, the optimal time is $T_{\text{ENT}'}(\frac{\pi}{4}) = \frac{\pi}{4\sqrt{2}\omega}$ whereas $T_{\text{ENT}}(\frac{\pi}{4}) = \frac{\sqrt{7}\pi}{4\sqrt{2}\omega}$. The difference comes from the relative phase between $|00\rangle$ and $|11\rangle$ in the final state. On the other hand, the case $\varphi = \pi$ corresponds to the same operation and $T_{\text{ENT}'}(\pi) = T_{\text{ENT}}(\pi)$.

4.4 Dynamical or static

In Section 4.1, we have seen that if there is no constraint except the normalization of the Hamiltonian, static Hamiltonians are obtained as the solution of the quantum brachistochrone. Any unitary operator can be generated by static Hamiltonians.

The time-optimal Hamiltonian for generating SWAP gate can be also obtained by diagonalizing U_{SWAP} :

$$U_{\text{SWAP}} = e^{i\chi} W \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} W^\dagger, \quad W = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \\ 0 & \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}. \quad (4.110)$$

This leads to the exponential form:

$$U_{\text{SWAP}} = \exp[-iW \text{diag}(-\chi, -\chi, \pm\pi - \chi, -\chi)W^\dagger], \quad (4.111)$$

which can be written in terms of the static Hamiltonian: $U_{\text{SWAP}} = \exp[-iHT]$. To minimize $\text{Tr}(HT)^2$, we choose $\chi = \pm\frac{\pi}{4}$ and obtain

$$HT = \pm\frac{\pi}{4} \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \quad (4.112)$$

which coincides with (4.74). On the other hand, by the same calculation, the entangler gate U_{ENT} becomes

$$U_{\text{ENT}} = \exp[-iHT], \quad HT = \begin{bmatrix} 0 & 0 & 0 & -i\varphi \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ i\varphi & 0 & 0 & 0 \end{bmatrix}, \quad (4.113)$$

which cannot be written by the restricted Hamiltonian (4.19). This is a reason why the solution for the entangler gate (4.107) is dynamical. The

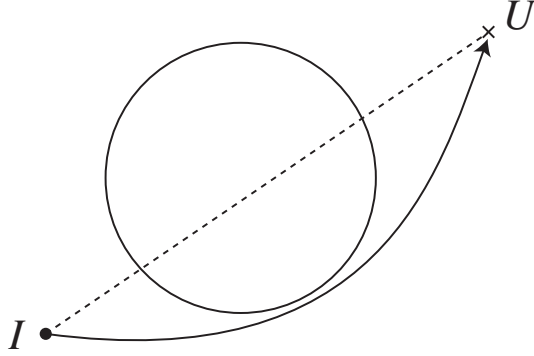


Figure 4.4: If there is no obstacle (circle) due to the restriction of the system, we can go straight (dotted line) by the constant Hamiltonian. Otherwise we have to use a dynamical Hamiltonian (curve).

quantum brachistochrone equation gives the dynamical or static Hamiltonian as the optimal solution depending on the constraint of the system and the target unitary operator.

4.5 Discussion

On the restricted system, the unitary operation U is generated by a dynamical Hamiltonian $H(t)$ in general. This can be written as $U = U_M U_{M-1} \cdots U_1$ with $U_m = \exp[-iH(t_m)\Delta t_m]$ where Δt_m is infinitesimal and $t_m = \sum_{k=1}^m \Delta t_k$. By choosing $\text{Tr } H^2 = N\omega^2$, where ω is a constant and N is dimension of the

Hilbert space, any traceless Hamiltonian can be written as

$$H = \omega \sum_k n_k \sigma_k = \omega \mathbf{n} \cdot \boldsymbol{\sigma} \quad (4.114)$$

where σ_k , ($k = 1, \dots, N^2 - 1$) is an orthonormal basis for $N \times N$ Hermitian matrices on the Hilbert-Schmidt inner product, i.e. $\text{Tr} \sigma_i \sigma_j = N \delta_{ij}$, and coefficients n_k are real. By using this notation, the normalization constraint (4.2) can be seen as $\sum_k n_k^2 = 1$ and the unitary operator is written as

$$U_m = \exp[-i(\omega \Delta t_m) \mathbf{n} \cdot \boldsymbol{\sigma}]. \quad (4.115)$$

We can see that the normalization constraint for the Hamiltonian defines the available action per a unit of time. To quantify the amount of time for generating a unitary operation U with a constant ω , namely $\omega T = \sum_m \omega \Delta t_m$, is equivalent to quantification of the action $\sum_m \omega(t_m) \Delta t_m$ where $\omega^2(t) = \frac{1}{N} \text{Tr} H^2(t)$. Thus, the optimal time to generate a unitary operation U_{target} with the normalization constraint for the Hamiltonian can be seen as the minimal action required to make U_{target} on a given system.

It is also possible to quantify a part of the effect of Hamiltonian by choosing appropriate constraint instead of (4.2) depending on the purpose, which is related to the work by Nielsen *et al.* [44, 45, 46] (see Appendix B).

An example for the case that the constraint is imposed by inequalities is in Appendix C, in which we consider the quantum dot model.

4.6 Summary

We have solved the quantum brachistochrone problem for some simple models analytically, in which we have derived a general solution and fixed integration constants by equating the target and the solution up to phase. The optimal solution is found by choosing the set of constants which minimizes the duration time. The quantum brachistochrone gives the dynamical or static Hamiltonian depending on the restriction for the system and the choice of the target. To fix the unit of time, we have used the normalization constraint (4.2). The meaning of this quantification is discussed in Section 4.5.

The problem for the time-optimal unitary operations are solved for a simple model. It has greater relevance for quantum computation, since we need to prepare unitary operations as building blocks for the quantum computer regardless of initial states which is unknown during a computation in general.

In this chapter, we find the way to make the target exactly. But in some cases, we do not need the exact target. The required time will be reduced when we set the final condition for the fidelity to the target lower than one. We can also consider the problem to maximize the fidelity to the target by optimizing the control in a fixed time.

Chapter 5

Simulated annealing method

The simulated annealing method is a stochastic search algorithm which is used for finding the global minimum of a function of “energy” whose structure is complex or not smooth in the region. A single step of the annealing process is random walks determined by so called Metropolis criterion. If we find the point with lower energy than before, we must take a step there, otherwise we can still take a step with the probability determined by the Boltzmann distribution,

$$p_{i+1} = \begin{cases} 1 & \text{if } E_{i+1} < E_i \\ e^{-\frac{E_{i+1}-E_i}{kT}} & \text{otherwise,} \end{cases} \quad (5.1)$$

where k is the “Boltzmann constant” and T is the “temperature”. The annealing is proceeded by gradually reducing the temperature with the factor μ_T and taking steps. By choosing smaller reducing factor $\mu_T \geq 1$ of the temperature, one can achieve the global minimum with higher probability.

Whereas Newton’s method cannot avoid being trapped in local minima, this method can escape from them, because it can take a step into a point with higher energy than before with a certain probability.

For our quantum brachistochrone problem, we choose 1-(fidelity) as the “energy”, in the annealing process, to minimize the distance between the target U_{target} and the time-optimal path of the unitary operator generated by the Schrödinger equation with the dynamical Hamiltonian governed by the quantum brachistochrone equation. The duration time to generate a unitary operation close to the target is found in the certain computational range of the time (see figure 5.1). For unitary operators acting on N dimensional Hilbert space, we will call the function $f(U_1, U_2) = \frac{1}{N} |\text{Tr } U_1^\dagger U_2|$ fidelity.

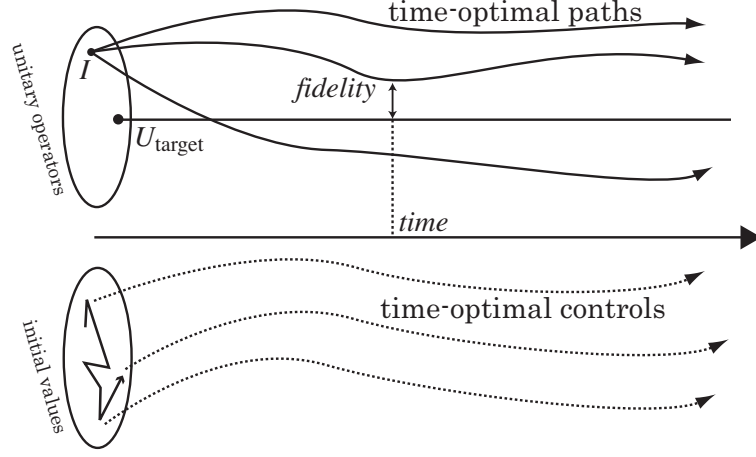


Figure 5.1: Time-optimal paths in the space of unitary operators are generated by the Schrödinger equation with dynamical Hamiltonian governed by the quantum brachistochrone equation whose initial values are given by the random walks in the simulated annealing process. The “energy” in the annealing process is chosen to the 1-(fidelity) between the target and a closest point of a time-optimal path in the certain range of the time duration.

5.1 Interacting two 1/2 spins

Let us consider the two-qubit system that has the Hamiltonian

$$H = J\boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^2 + \mathbf{B}^1(t) \cdot \boldsymbol{\sigma}^1 + \mathbf{B}^2(t) \cdot \boldsymbol{\sigma}^2 \quad (5.2)$$

with constants J and $\text{Tr } H^2 = 4\Omega^2$ which implies

$$\Omega^2 = 3J^2 + \omega^2 \quad (5.3)$$

$$\omega^2 = |\mathbf{B}^1|^2 + |\mathbf{B}^2|^2. \quad (5.4)$$

Those constraints are represented by following constraint operator

$$F = \lambda_{ij}\sigma_i \otimes \sigma_j + \mu H \quad (5.5)$$

$$= (\lambda_{ij} + J\mu\delta_{ij})\sigma_i \otimes \sigma_j + \mu B_i^1 \sigma_i \otimes I + \mu B_i^2 I \otimes \sigma_i \quad (5.6)$$

where λ_{ij} and μ are Lagrange multipliers.

5.1.1 Quantum brachistochrone equation

The time-optimal control sequence of external fields $\mathbf{B}^1(t)$ and $\mathbf{B}^2(t)$ is obtained by solving the quantum brachistochrone equation $i\dot{F} = [H, F]$. In this model, each side of the equation are written as

$$i\dot{F} = i\frac{d}{dt}(\lambda_{ij} + J\mu\delta_{ij})\sigma_i \otimes \sigma_j + \frac{d}{dt}(\mu B_i^1)\sigma_i \otimes I + \frac{d}{dt}(\mu B_i^2)I \otimes \sigma_i \quad (5.7)$$

$$[H, F] = 2i\{J\epsilon_{ijk}\lambda_{ij}(-\sigma_k \otimes I + I \otimes \sigma_k) + \epsilon_{lki}B_l^1\lambda_{ij}\sigma_k \otimes \sigma_j + \epsilon_{ljk}B_l^2\lambda_{ij}\sigma_i \otimes \sigma_k\}. \quad (5.8)$$

Using the orthogonality of Pauli matrices in Hilbert-Schmidt inner product $\langle A, B \rangle = \text{Tr}(AB)$, we obtain

$$\dot{\mu}B_i^1 + \mu\dot{B}_i^1 = -2J\epsilon_{ijk}\lambda_{jk} \quad (5.9)$$

$$\dot{\mu}B_i^2 + \mu\dot{B}_i^2 = 2J\epsilon_{ijk}\lambda_{jk} \quad (5.10)$$

$$\dot{\lambda}_{ij} + J\dot{\mu}\delta_{ij} = 2(\epsilon_{lki}B_l^1\lambda_{kj} + \epsilon_{lkj}B_l^2\lambda_{ik}). \quad (5.11)$$

Equation (5.9) and (5.10) leads to

$$\dot{\mu}\mathbf{B} + \mu\dot{\mathbf{B}} = \mathbf{0} \quad (5.12)$$

$$\dot{\mu}\mathbf{D} + \mu\dot{\mathbf{D}} = -4J\mathbf{L} \quad (5.13)$$

where $\mathbf{B} = \mathbf{B}^1 + \mathbf{B}^2$, $\mathbf{D} = \mathbf{B}^1 - \mathbf{B}^2$ and

$$L_i = \epsilon_{ijk}\lambda_{jk}. \quad (5.14)$$

Without loss of generality, it is possible to put

$$\mathbf{B}(t) = B(t)\mathbf{e}_z, \quad (5.15)$$

since the system has the rotational symmetry and (5.12) fixes the direction of $\mathbf{B}$. Taking a summation of inner products of B_i^1 with (5.9) and B_i^2 with (5.10), we get

$$\dot{\mu} = -\frac{2J}{\omega^2}\mathbf{D} \cdot \mathbf{L}. \quad (5.16)$$

5.1.2 Result of the numerical computation

Using the simulated annealing method, we realized a control sequence to give the CNOT gate numerically. The optimal-time given by a numerical computation is $T_{\text{CNOT}} = 3.44$ with the choice $J = 1.0$ and $\omega = 1.0$, which can be comparable to the solution $T_{\text{CNOT}} = \frac{\pi}{4J} \simeq 0.79$ derived by Zhang *et al.* [19]. In their model, one qubit operations can be done instantaneously, namely the strength of one qubit operations is assumed to be large enough to compare with the coupling strength between two qubits. This result indicates one can implement two qubit gate (entangler gate) without strong one qubit operations nor long duration time for interactions.

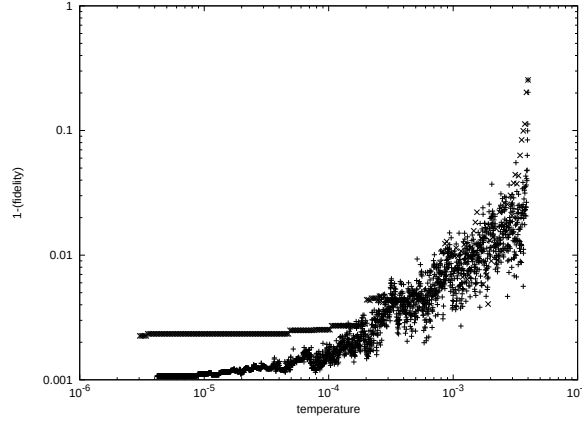


Figure 5.2: The fidelity of the numerical solution to the target is enhanced during the annealing process in which the temperature is gradually reduced (from upper right to lower left). The process with the dumping factor $\mu_T = 1.003$ is indicated as red points and $\mu_T = 1.03$ is indicated as green points. A process with lower dumping factor can give a solution with higher quality. The lowest value is $1 - f(U(T), U_{\text{CNOT}}) = 1.07 \times 10^{-3}$ at 2291th step.

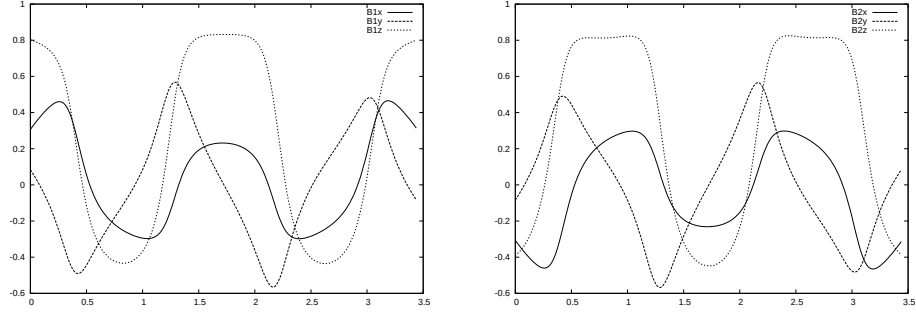


Figure 5.3: The time-optimal control for the parameters, which generates CNOT gate.

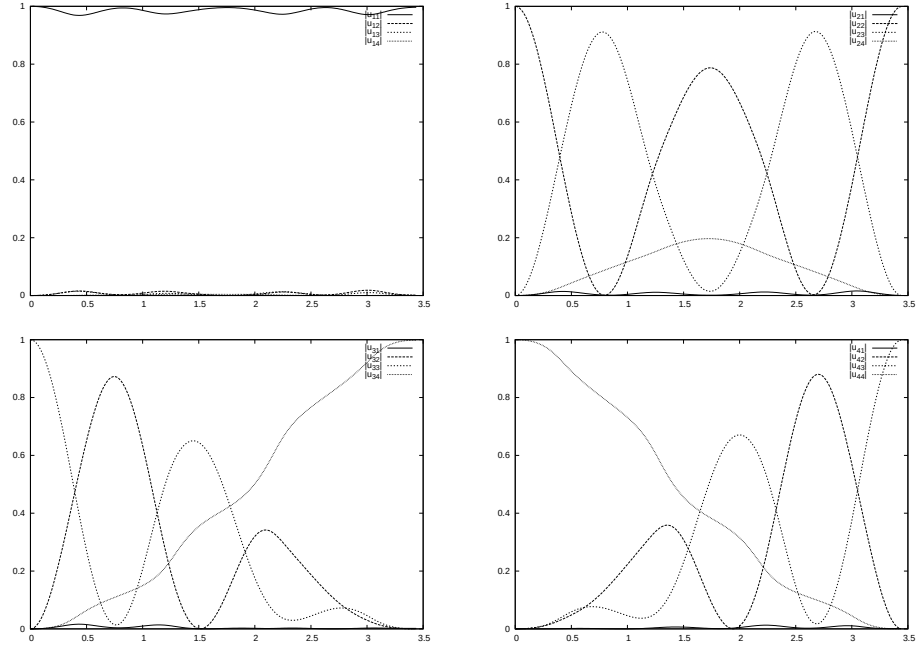


Figure 5.4: The evolution of the unitary matrix from I toward U_{CNOT} . $|u_{11}|$, $|u_{22}|$, $|u_{34}|$ and $|u_{43}|$ converge at unity.

5.2 Superconducting flux qubits

We choose as an example the following coupled two-qubit Hamiltonian,

$$H = -J(t)\sigma_x \otimes \sigma_x + \Delta_1(t)\sigma_z \otimes I + \Delta_2(t)I \otimes \sigma_z + \epsilon_1(t)\sigma_x \otimes I + \epsilon_2(t)I \otimes \sigma_x \quad (5.17)$$

with the constraint $J^2 + \Delta_1^2 + \Delta_2^2 + \epsilon_1^2 + \epsilon_2^2 = \omega^2 = \text{constant}$. The quantum brachistochrone equation $i\dot{F} = [H, F]$ gives the time-optimal manipulation of the parameters in the Hamiltonian. According to the section 3.4, the operator F is defined as

$$F = H + \sum_{(i,j) \neq (x,x)} \lambda_{ij} \sigma_i \otimes \sigma_j + \eta_1 \sigma_y \otimes I + \eta_2 I \otimes \sigma_y \quad (5.18)$$

where η_i and λ_{ij} are Lagrange multipliers.

5.2.1 Equations

Equation (5.18) can be decomposed to the following simultaneous first-order differential equations,

$$\dot{\epsilon}_1 = -2\Delta_1\eta_1 \quad (5.19)$$

$$\dot{\epsilon}_2 = -2\Delta_2\eta_2 \quad (5.20)$$

$$\dot{\Delta}_1 = -2(J\lambda_{yx} - \epsilon_1\eta_1) \quad (5.21)$$

$$\dot{\Delta}_2 = -2(J\lambda_{xy} - \epsilon_2\eta_2) \quad (5.22)$$

$$\dot{J} = 2(\Delta_1\lambda_{yx} + \Delta_2\lambda_{xy}) \quad (5.23)$$

$$\dot{\eta}_1 = 2J\lambda_{zx} \quad (5.24)$$

$$\dot{\eta}_2 = 2J\lambda_{xz} \quad (5.25)$$

$$\dot{\lambda}_{xy} = -2(\Delta_1\lambda_{yy} + \epsilon_2\lambda_{xz}) \quad (5.26)$$

$$\dot{\lambda}_{yx} = -2(\Delta_2\lambda_{yy} + \epsilon_2\lambda_{zx}) \quad (5.27)$$

$$\dot{\lambda}_{yz} = 2(\Delta_1\lambda_{xz} - \epsilon_1\lambda_{zz} + \epsilon_2\lambda_{yy}) \quad (5.28)$$

$$\dot{\lambda}_{zy} = 2(\Delta_2\lambda_{zx} + \epsilon_1\lambda_{yy} - \epsilon_2\lambda_{zz}) \quad (5.29)$$

$$\dot{\lambda}_{zx} = 2(-J\eta_1 - \Delta_2\lambda_{zy} + \epsilon_1\lambda_{yx}) \quad (5.30)$$

$$\dot{\lambda}_{xz} = 2(-J\eta_2 - \Delta_1\lambda_{yz} + \epsilon_2\lambda_{xy}) \quad (5.31)$$

$$\dot{\lambda}_{yy} = 2(\Delta_1\lambda_{xy} + \Delta_2\lambda_{yx} - \epsilon_1\lambda_{zy} - \epsilon_2\lambda_{yz}) \quad (5.32)$$

$$\dot{\lambda}_{zz} = 2(\epsilon_1\lambda_{yz} + \epsilon_2\lambda_{zy}). \quad (5.33)$$

An initial condition for 15 variables $\{\epsilon_i, \Delta_i, J, \eta_i, \lambda_{ij}\}$, gives a time-optimal evolution of the Hamiltonian $H(t)$ and the corresponding unitary operator $U(t) = \mathcal{T} \exp(-i \int H(t) dt)$. The remaining problem is to find the initial condition which gives the desired unitary operator U_{target} .

5.2.2 Numerical analysis

We solve this problem by using the simulated annealing algorithm which can efficiently avoid local minima. The dimension of the parameter space is 16: the initial condition for 15 variables and the product ωT . Integrating (5.19)-(5.33) and the Schrödinger equation with an initial condition, we get a numerical solution of the unitary $U(T)$. The distance between the numerical solution and the target is measured by the quantity $d = 1 - f = 1 - \frac{1}{4} |\text{Tr}[U_{\text{target}}^\dagger U(T)]|$ which is used as the energy and minimized by the annealing process.

For instance, we choose the CNOT gate as the target. By 50 evaluations for each step of the reduction of the temperature in the annealing process, we get the unitary with $q = 0.99341$ and $\omega T = 7.93$.

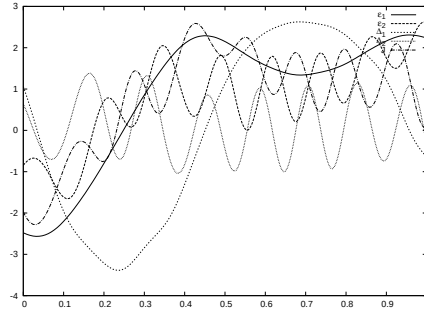


Figure 5.5: The time-optimal manipulation for the parameters.

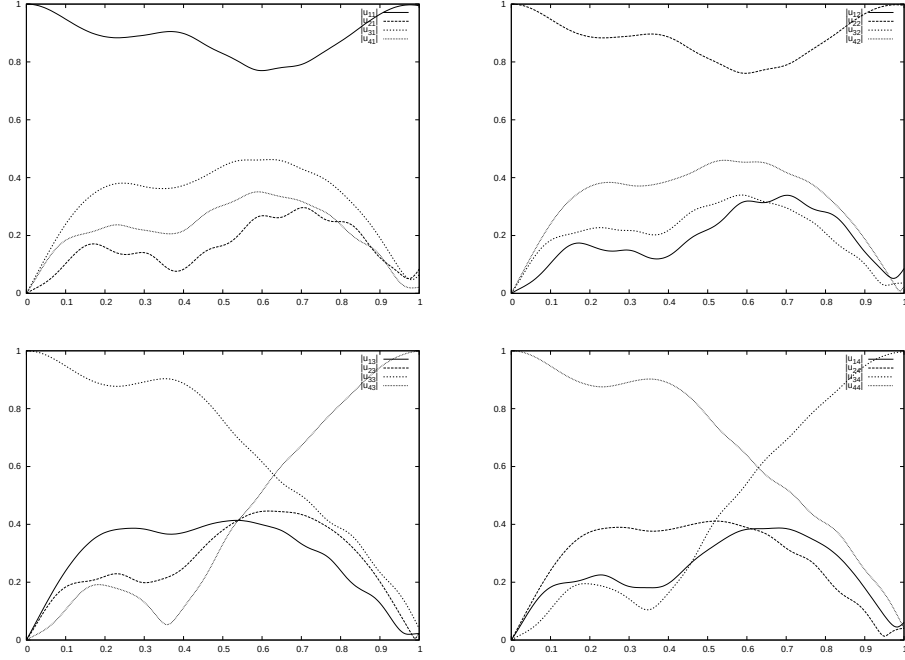


Figure 5.6: The evolution of the unitary matrix from I toward U_{CNOT} . $|u_{11}|$, $|u_{22}|$, $|u_{34}|$ and $|u_{43}|$ are approaching to 1.

5.3 Summary

We have seen the application of the simulated annealing method to the quantum brachistochrone with two physical models whose analytic solutions have not been found. This method requires the analytic form of N^2 equations given by the quantum brachistochrone equation for the system with $\mathcal{H}_N$. The quality of the solution can be improved by choosing large step number and small dumping factor.

Chapter 6

The Krotov method

Tannor *et al.* showed an iterative method to find an optimal control based on the Krotov method [29, 30]. Rabitz *et al.* provides a general framework for designing controls over molecular dynamics phenomena to maximize an expectation value e.g. the occupation number of a state or the fidelity to a target wave packet. Palao and Kosloff applied this method to find the optimal way to control unitary transformations [31]. Their studies are not for time-optimal control but can be modified to find it.

6.1 Formalism

In this section, the quantum optimal control theory [17, 28] is reviewed. The quantum system is assumed to have controllable parameters $\varepsilon_k(t)$ in the Hamiltonian

$$H(\{\varepsilon_k(t)\}) = H_0 + \sum_k \varepsilon_k(t) \sigma_k. \quad (6.1)$$

The problem is to find a control $\{\varepsilon_k(t)\}$ for $t \in [0, T]$, which steers the given initial state $|\psi_i\rangle$ to a final state and yields the expectation value of some operator O as much as possible with small amount of external fields. The whole cost is evaluated by the summation of two components

$$J_1 = \langle \psi(T) | O | \psi(T) \rangle \quad (6.2)$$

$$J_2 = - \sum_k \gamma_k \int \varepsilon_k^2(t) dt. \quad (6.3)$$

where J_1 is desired to be large whereas the integral of the strength of external fields $-J_2$ to be small. The operator O in J_1 is chosen depending on the purpose. Positive factors γ_k in J_2 are the weight of each external field in the whole cost. The functional to be maximized is defined as

$$J = J_1 + J_2 - 2 \operatorname{Re} \left[\int_0^T dt \langle \phi | \left(\frac{d}{dt} + iH \right) | \psi \rangle \right], \quad (6.4)$$

By taking variation with respect to $|\phi\rangle$, the third term gives the Schrödinger equation

$$i \frac{d}{dt} |\psi(t)\rangle = H(t) |\psi(t)\rangle. \quad (6.5)$$

From the variation of $|\psi\rangle$, we obtain

$$i \frac{d}{dt} |\phi(t)\rangle = H |\phi(t)\rangle \quad (6.6)$$

$$|\phi(T)\rangle = O |\psi(T)\rangle. \quad (6.7)$$

The variation by ε_k yields

$$\varepsilon_k(t) = \frac{1}{\gamma_k} \operatorname{Im} \langle \phi(t) | \sigma_k | \psi(t) \rangle. \quad (6.8)$$

The problem is reduced to finding $|\phi(0)\rangle$ which meets (6.7), but it is still hard to solve in general.

6.2 Numerical procedure

There is a numerical method to solve this problem, which is reviewed in [32, 33, 34] as follows. As the first step, we guess the field $\varepsilon_k^{(0)}(t)$ and propagate initial state $|\psi_i\rangle$ by this field

$$|\psi^{(0)}(0)\rangle \xrightarrow{\varepsilon^{(0)}(t)} |\psi^{(0)}(T)\rangle \quad (6.9)$$

$$\varepsilon_k^{(0)} = 0, \text{ for example.} \quad (6.10)$$

Usually, the initial guess is taken as $\varepsilon_k^{(0)}(t) = 0$. The final condition for the Lagrange multiplier $|\phi\rangle$ is determined by (6.7), which can be propagated

backward from $|\phi^{(0)}(T)\rangle = O|\psi^{(0)}(T)\rangle$ to give $|\phi^{(0)}(0)\rangle$.

$$|\phi^{(0)}(0)\rangle \xleftarrow{\varepsilon^{(\frac{1}{2})}(t)} |\phi^{(0)}(T)\rangle \quad (6.11)$$

$$\varepsilon_k^{(\frac{1}{2})}(t) = \frac{1}{\gamma_k} \text{Im}\langle\phi^{(0)}(t)|\sigma_k|\psi^{(0)}(t)\rangle. \quad (6.12)$$

The i -th step is computed using the result of previous step $|\phi^{(i-1)}(t)\rangle$,

$$|\psi^{(i)}(0)\rangle \xrightarrow{\varepsilon^{(i)}(t)} |\psi^{(i)}(T)\rangle \quad (6.13)$$

$$\varepsilon_k^{(i)}(t) = \frac{1}{\gamma_k} \text{Im}\langle\phi^{(i-1)}(t)|\sigma_k|\psi^{(i)}(t)\rangle, \quad (6.14)$$

and using the final condition $|\phi^{(i)}(T)\rangle = O|\psi^{(i)}(T)\rangle$, we compute backward

$$|\phi^{(i)}(0)\rangle \xleftarrow{\varepsilon^{(i+\frac{1}{2})}(t)} |\phi^{(i)}(T)\rangle \quad (6.15)$$

$$\varepsilon_k^{(i)}(t) = \frac{1}{\gamma_k} \text{Im}\langle\phi^{(i)}(t)|\sigma_k|\psi^{(i)}(t)\rangle. \quad (6.16)$$

The convergence of this iteration is detected by the difference of the field $\int_0^T |\varepsilon^{(i)}(t) - \varepsilon^{(i-1)}(t)| dt$.

6.3 Application to the unitary evolution

The generalization for the optimization to the unitary operations is straightforward. To find the optimal control which maximizes the overlap between the generated unitary operator and the target $|\text{Tr } U_{\text{target}}^\dagger U(T)|$, we replace the functional (6.4) as

$$J = |\text{Tr } U_{\text{target}}^\dagger U(T)|^2 - 2 \text{Re} \int_0^T \text{Tr}[V^\dagger(t)(\frac{d}{dt} + iH(t))U(t)] dt - \sum_k \gamma_k \int_0^T \varepsilon_k^2(t) dt, \quad (6.17)$$

where γ_k are positive constants.

6.3.1 Convergence of the iterative method

In this section we present the scheme introduced by Tannor *et al.* [29] with modification to apply to the unitary evolution. Suppose we have a set of functions $\{U^{(i)}(t), V^{(i)}(t), \varepsilon^{(i)}(t)\}$ and make a step to $U^{(i+1)} = U^{(i)} + \Delta U$, $V^{(i+1)} =$

$V^{(i)} + \Delta V, \varepsilon^{(i+1)} = \varepsilon^{(i)} + \Delta \varepsilon$ so that incrementation of J to be positive. To evaluate the incrementation of the cost functional J , we decompose it into three parts

$$J^{(i+1)} - J^{(i)} = \Delta_V J + \Delta_\varepsilon J + \Delta_U J \quad (6.18)$$

$$\Delta_V J = J[U^{(i+1)}(t), V^{(i+1)}(t), \varepsilon^{(i+1)}(t)] - J[U^{(i+1)}(t), V^{(i)}(t), \varepsilon^{(i+1)}(t)] \quad (6.19)$$

$$\Delta_\varepsilon J = J[U^{(i+1)}(t), V^{(i)}(t), \varepsilon^{(i+1)}(t)] - J[U^{(i+1)}(t), V^{(i)}(t), \varepsilon^{(i)}(t)] \quad (6.20)$$

$$\Delta_U J = J[U^{(i+1)}(t), V^{(i)}(t), \varepsilon^{(i)}(t)] - J[U^{(i)}(t), V^{(i)}(t), \varepsilon^{(i)}(t)]. \quad (6.21)$$

For simplicity, we omit the suffix of ε_k which can be easily recovered. The first part comes from the update for the Lagrange multiplier function $V(t)$,

$$\Delta_V J = -2 \operatorname{Re} \int_0^T \operatorname{Tr}[\Delta V^\dagger(t) (\frac{d}{dt} + iH^{(i+1)}(t)) U^{(i+1)}] dt. \quad (6.22)$$

The action (6.17) can be partially integrated to be

$$J = G + \int_0^T R dt \quad (6.23)$$

where

$$G = |\operatorname{Tr} U_{\text{target}}^\dagger U(T)|^2 - 2[\operatorname{Re} \operatorname{Tr} V(t)^\dagger U(t)]_{t=0}^T \quad (6.24)$$

$$R = 2 \operatorname{Re} \operatorname{Tr}[(\dot{V}^\dagger(t) - V^\dagger(t)iH(t))U(t)] - \sum_k \gamma_k \varepsilon_k^2(t). \quad (6.25)$$

In this notation, $\Delta_\varepsilon J$ and $\Delta_U J$ are written as

$$\Delta_\varepsilon J = \int_0^T \Delta_\varepsilon R dt \quad (6.26)$$

$$\Delta_U J = \Delta_U G + \int_0^T \Delta_U R dt. \quad (6.27)$$

For fixed $U(0)$, $\Delta_U G$ is

$$\begin{aligned} \Delta_U G &= G(U^{(i+1)}(T), V^{(i)}(T)) - G(U^{(i)}(T), V^{(i)}(T)) \\ &= |\operatorname{Tr} U_{\text{target}}^\dagger \Delta U(T)|^2 + 2 \operatorname{Re}\{(\operatorname{Tr} U_{\text{target}}^\dagger U^{(i)}(T))^* \operatorname{Tr} U_{\text{target}}^\dagger \Delta U - \operatorname{Tr} V^{(i)\dagger} \Delta U\}. \end{aligned} \quad (6.28)$$

The part for ε is quadratic of $\Delta\varepsilon$

$$\Delta_\varepsilon R = R(U^{(i+1)}, V^{(i)}, \varepsilon^{(i+1)}) - R(U^{(i+1)}, V^{(i)}, \varepsilon^{(i)}) \quad (6.29)$$

$$= -2 \operatorname{Re} \operatorname{Tr}(V^{(i)\dagger} i \sigma U^{(i+1)}) \Delta\varepsilon - \gamma(2\varepsilon^{(i)} \Delta\varepsilon + \Delta\varepsilon^2) \quad (6.30)$$

$$= -\gamma(\varepsilon^{(i+1)} - \frac{1}{\gamma} \operatorname{Im} \operatorname{Tr} V^{(i)\dagger} \sigma U^{(i+1)})^2 + \gamma(\varepsilon^{(i)} - \frac{1}{\gamma} \operatorname{Im} \operatorname{Tr} V^{(i)\dagger} \sigma U^{(i+1)})^2, \quad (6.31)$$

and the part for $U(t)$ is

$$\Delta_U R = R(U^{(i+1)}, V^{(i)}, \varepsilon^{(i)}) - R(U^{(i)}, V^{(i)}, \varepsilon^{(i)}) \quad (6.32)$$

$$= 2 \operatorname{Re} \operatorname{Tr}(\dot{V}^{(i)\dagger} - V^{(i)\dagger} i H^{(i)}) \Delta U. \quad (6.33)$$

An easy choice which makes the incrementation positive is

$$V^{(i)}(T) = (\operatorname{Tr} U_{\text{target}}^\dagger U^{(i)}(T)) U_{\text{target}} \quad (6.34)$$

$$i\dot{V}^{(i)}(t) = \left(H_0 + \sum_k \varepsilon_k^{(i)}(t) \sigma_k \right) V^{(i)}(t) \quad (6.35)$$

$$i\dot{U}^{(i+1)}(t) = \left(H_0 + \sum_k \varepsilon_k^{(i+1)}(t) \sigma_k \right) U^{(i+1)}(t), \quad (6.36)$$

$$\varepsilon^{(i+1)}(t) = \frac{1}{\gamma} \operatorname{Im} \operatorname{Tr} V^{(i)\dagger}(t) \sigma U^{(i+1)}(t) \quad (6.37)$$

and the corresponding incrementation is

$$\Delta J = |\operatorname{Tr} U_{\text{target}}^\dagger \Delta U(T)|^2 + \gamma \int_0^T \Delta\varepsilon^2 dt \geq 0. \quad (6.38)$$

The other possible choice, which is known to be more efficient [33] and explained in previous section, is

$$V^{(i)}(T) = (\operatorname{Tr} U_{\text{target}}^\dagger U^{(i)}(T)) U_{\text{target}} \quad (6.39)$$

$$i\dot{V}^{(i)}(t) = \left(H_0 + \sum_k \varepsilon_k^{(i+\frac{1}{2})}(t) \sigma_k \right) V^{(i)}(t) \quad (6.40)$$

$$\varepsilon^{(i+\frac{1}{2})}(t) = \frac{1}{\gamma} \operatorname{Im} \operatorname{Tr} V^{(i)\dagger}(t) \sigma U^{(i)}(t) \quad (6.41)$$

$$i\dot{U}^{(i+1)}(t) = \left(H_0 + \sum_k \varepsilon_k^{(i+1)}(t) \sigma_k \right) U^{(i+1)}(t) \quad (6.42)$$

$$\varepsilon^{(i+1)}(t) = \frac{1}{\gamma} \operatorname{Im} \operatorname{Tr} V^{(i)\dagger}(t) \sigma U^{(i+1)}(t). \quad (6.43)$$

In this choice, the function $V^{(i)}(t)$ is obtained by solving the non-linear equation (6.40) backward with the parameter (6.41) from the boundary condition (6.39), in which the function $U^{(i)}(t)$ given in the previous step is used. And (6.43) gives next function $U^{(i+1)}(t)$ through the non-linear equation (6.42) in which the function $V^{(i)}(t)$ obtained in the previous step is used. The corresponding incrementations are

$$\Delta_U R = -2 \operatorname{Im} \operatorname{Tr}[V^{(i)\dagger}(H^{(i+\frac{1}{2})} - H^{(i)})\Delta U] = 2\gamma(\varepsilon^{(i)} - \varepsilon^{(i+\frac{1}{2})})(\varepsilon^{(i+1)} - \varepsilon^{(i+\frac{1}{2})}) \quad (6.44)$$

$$\Delta_\varepsilon R = \gamma(\varepsilon^{(i+1)} - \varepsilon^{(i)})^2, \quad (6.45)$$

thus we have

$$\Delta J = |\operatorname{Tr} U_{\text{target}}^\dagger \Delta U(T)|^2 + \gamma \int_0^T \{(\varepsilon^{(i+1)} - \varepsilon^{(i+\frac{1}{2})})^2 + (\varepsilon^{(i)} - \varepsilon^{(i+\frac{1}{2})})^2\} dt \geq 0. \quad (6.46)$$

The optimal solution maximizes the cost functional J . This indicates that the functions will be getting closer to the optimal solution by every iteration procedure. In practice, the incrementation ΔJ will converge to zero, which means that the functions $\{U^{(i)}, V^{(i)}, \varepsilon^{(i)}\}$ converges to a solution of the Euler-Lagrange equation derived by the calculus of variation for the functional J .

6.3.2 Accuracy

To compute the Krotov method in practice, we have to solve the differential equation as a difference equation and store the time evolution in a finite amount of memory. The time is divided into S steps and the cost functional J is regarded to be converged if $\Delta J \leq \epsilon$. To see the effect of the step size S and the threshold ϵ for the result, we carry out the trial numerical computations to some cases. The figure (6.1) indicates that the case with lower quality is affordable just to see the tendency of the relation between the duration time and the fidelity.

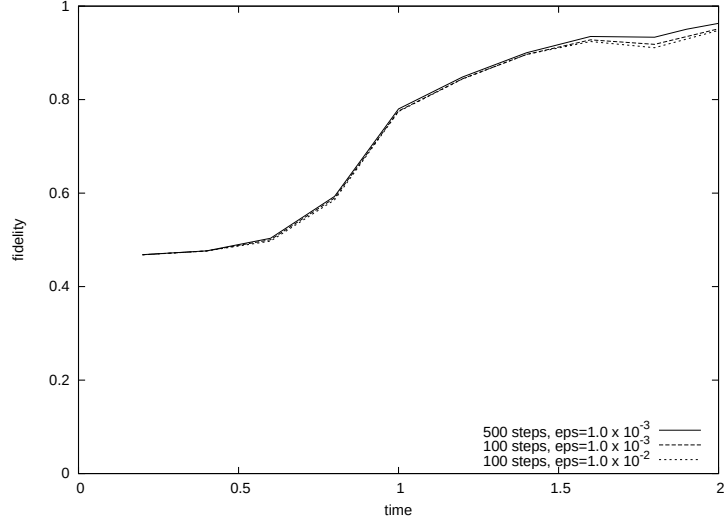


Figure 6.1: The results of the Krotov method for cases $(S = 500, \epsilon = 1.0 \times 10^{-3})$, $(S = 100, \epsilon = 1.0 \times 10^{-3})$ and $(S = 100, \epsilon = 1.0 \times 10^{-2})$, where S is a number of time steps and ϵ is a threshold for detecting the convergence of the cost functional. The Hamiltonian is $H = J\sigma_z^1\sigma_z^2 + \mathbf{B}^1 \cdot \boldsymbol{\sigma}^1 + \mathbf{B}^2 \cdot \boldsymbol{\sigma}^2$ where the coupling constant is $J = 1.0$. The target is two-qubit QFT gate. The penalty factor is $\gamma = 1.0$.

6.4 Application to the time-optimal control

There are a couple of ways to treat the time-optimal control problem in Krotov's scheme, which can be done by some modifications for the original scheme. One is to consider the fidelity optimization problem for several time durations $T_1, T_2, \dots$, and find the convergence of the optimal fidelities. The shortest time to give a unitary gate which has a sufficiently large fidelity to the target can be regarded as the optimal time.

The other is to consider the modification of the Hamiltonian which admits every coefficient of components in the Hamiltonian to be a variable. After we obtain a solution for the modified Hamiltonian, we reparameterize and scale it to make the coefficient of the static term unity. The priority of the duration time in the whole cost is defined by the penalty factor.

In both cases, the duration time is optimized as a part of a cost function

consists of some components, e.g., the fidelity to the target, the fluence of the fields.

To consider the minimization of the duration time solely, we have to impose constraints on the field and exclude them from the cost function. By imposing the constraint, we can consider the application of the Krotov method to our model discussed in Chapter 4.

6.4.1 Fidelity optimal control

Suppose we want to find the control to give a unitary gate close to the target U_{target} as much fidelity as possible in a fixed duration time T . The cost functional can be formulated as

$$J = J_1 + J_2 - 2 \operatorname{Re} \left[\int_0^T dt \operatorname{Tr} V^\dagger \left\{ \frac{dU}{d\tau} + iHU \right\} \right], \quad (6.47)$$

$$J_1 = |\operatorname{Tr}(U_{\text{target}}^\dagger U(T))|^2 \quad (6.48)$$

$$J_2 = -\gamma \int_0^T dt \sum_k \varepsilon_k^2 \quad (6.49)$$

in which the penalty factor γ is chosen to be equal for all components of external fields. By solving the problem for many choice of duration times $T_1, T_2, \dots$, we obtain a profile of the relation between a given time T_i and the optimal fidelity $f(T_i)$ of attainable unitary to the target within the time. This relation can also be seen as the optimal time to obtain a unitary at a given fidelity range $T(f)$.

For the computation by this functional, we have to choose a penalty factor in advance which determines the ratio of the priority of the fidelity and the fluence (the integral of the strength of fields) in the cost functional. This choice of the penalty factor is artificial and the resultant cost is unknown in advance. If we want to seek a more efficient control than known control sequences, this penalty approach can be useful. But if we want to compare efficiency of models or to see some physical insight, this approach is too ambiguous because we do not know what is a reasonable choice of the penalty factor. An alternative way is to impose a natural constraint.

6.4.2 Low cost control

Suppose we have a quantum system with the Hamiltonian

$$H(t) = H_0 + \sum_k \varepsilon_k(t) \sigma_k, \quad (6.50)$$

where $\varepsilon_k(t)$ is controllable. The static term H_0 characterizes the time scale of this model. To consider the minimization of time in Krotov's scheme, we define a modified Hamiltonian

$$\tilde{H}(\tau) = \alpha(\tau) H_0 + \sum_k \tilde{\varepsilon}_k(\tau) \sigma_k \quad (6.51)$$

with positive function $\alpha(\tau)$ in a range $0 \leq \tau \leq \tau_1$. It generates a unitary operation

$$U_1 = \mathcal{T} \exp \left[-i \int_0^{\tau_1} \tilde{H}(\tau) d\tau \right]. \quad (6.52)$$

The cost is evaluated by the sum of two functional

$$J_1 = |\text{Tr}(U_{\text{target}}^\dagger U(\tau_1))|^2 \quad (6.53)$$

$$\text{and } J_2 = -\gamma_0 \int_0^{\tau_1} \alpha^2(\tau) d\tau - \sum_k \gamma_k \int_0^{\tau_1} \tilde{\varepsilon}_k^2(\tau) d\tau \quad (6.54)$$

where γ_0 and γ_k are the penalty factor to adjust the relative weight of each cost. The real time duration T can be derived by changing the integral parameter $dt = \alpha(\tau) d\tau$, which leads

$$U_1 = \mathcal{T} \exp \left[-i \int_0^{\tau_1} \left(\alpha(\tau) H_0 + \sum_k \tilde{\varepsilon}_k(\tau) \sigma_k \right) d\tau \right] \quad (6.55)$$

$$= \mathcal{T} \exp \left[-i \int_0^T \left(H_0 + \sum_k \frac{\tilde{\varepsilon}_k}{\alpha} \sigma_k \right) dt \right], \quad (6.56)$$

thus the optimal control is $\varepsilon(t) = \tilde{\varepsilon}(\tau(t))/\alpha(\tau(t))$, where $\tau(t)$ is a one-to-one function given by

$$t = \int_0^{\tau(t)} \alpha(\tau') d\tau' \quad (6.57)$$

since $\alpha(\tau) \geq 0$. We can solve the the optimal control problem for the sum of functionals (6.53) and (6.54) in the Krotov method by the action

$$J = |\text{Tr}(U_{\text{target}}^\dagger U_1)|^2 - \int_0^{\tau_1} d\tau \left(\gamma_0 \alpha^2 + \sum_k \gamma_k \tilde{\varepsilon}_k^2 \right) - 2 \text{Re} \left[\int_0^{\tau_1} d\tau \text{Tr} V^\dagger \left\{ \frac{dU}{d\tau} + i\tilde{H}U \right\} \right], \quad (6.58)$$

where $\tilde{\varepsilon}_k = \alpha \varepsilon_k$ and $\tilde{H} = \alpha(t)H_0 + \sum_k \tilde{\varepsilon}_k(t)\sigma_k$. The first and the second term are the functional which will be maximized. The third term restricts the evolution to obey the Schrödinger equation. The duration time is derived by $T = \int_0^{\tau_1} \alpha(\tau) d\tau$, which depends on the choice of penalty factors.

6.4.3 Constraints

We can impose a constraint for the external field $\sum_k \varepsilon_k^2 = \omega^2$ with a constant ω , which requires the second part of the cost functional to be

$$J_2 = - \int_0^T \gamma(t) \left(\sum_k (\varepsilon_k(t))^2 - \omega^2 \right) dt. \quad (6.59)$$

The demerit of this constraint is that the ratio between the strength of static component H_0 and the strength of controllable components ω is fixed. In this case, the parameter ε_k and a Lagrange multiplier γ are derived as

$$\varepsilon_k(t) = \frac{1}{\gamma} \text{Im Tr } V^\dagger \sigma_k U, \quad \gamma(t) = \frac{1}{\omega} \sqrt{\sum_k (\text{Im Tr } V^\dagger \sigma_k U)^2}. \quad (6.60)$$

In the iterative computation, these functions for the i -th step are obtained by

$$(6.37) \rightarrow \varepsilon_k^{(i+1)}(t) = \frac{1}{\gamma^{(i+1)}} \text{Im Tr } V^{(i)\dagger} \sigma_k U^{(i+1)}, \quad (6.61)$$

$$\gamma^{(i+1)}(t) = \frac{1}{\omega} \sqrt{\sum_k (\text{Im Tr } V^{(i)\dagger} \sigma_k U^{(i+1)})^2}. \quad (6.62)$$

This modification does not change the convergence behavior considered in Section 6.3.1, because of $J_2^{(i+1)} - J_2^{(i)} = - \int_0^T \gamma^{(i+1)} \sum_k ((\varepsilon_k^{(i+1)})^2 - (\varepsilon_k^{(i)})^2) dt$, which is the same form as the last term in (6.30).

In some cases, the spectral property of the external fields has restrictions (e.g. [8]), for example one cannot switch on and off arbitrarily or the frequency of the microwave imposed on the qubits are restricted in a certain range. Those conditions can be introduced in the numerical procedure by the filtering technique explained in Appendix E.

6.4.4 Output recycling

To plot the fidelity-time relation, the computations of the Krotov iteration for many time ranges are required. In this recursive computation, it is possible to use the result of the previous iteration process for the next process,

$$\varepsilon^{\text{next}(0)}(t) = \varepsilon^{\text{prev}(k_{\text{last}})}(t) \quad (6.63)$$

instead of choosing $\varepsilon^{(0)}(t) = 0$. This technique reduces the computational cost, if the optimal field profile for a time duration $T + \Delta T$ exists in the neighbor of that for a time duration T .

6.5 Comparison with the analytic solution

We have studied the coupled two-qubit model in Section 4.3 and obtained the analytic solutions for some targets. To see the accuracy, we compare the analytic solution and the numerical solution given by the Krotov method. As an example, we choose the swap gate. To solve the time optimization problem studied in Section 4.3, we choose the way considered in Section 6.4.1 and use the constraint (6.59) instead of (6.49). The result is shown in the figure 6.2, where the agreement seems perfect.

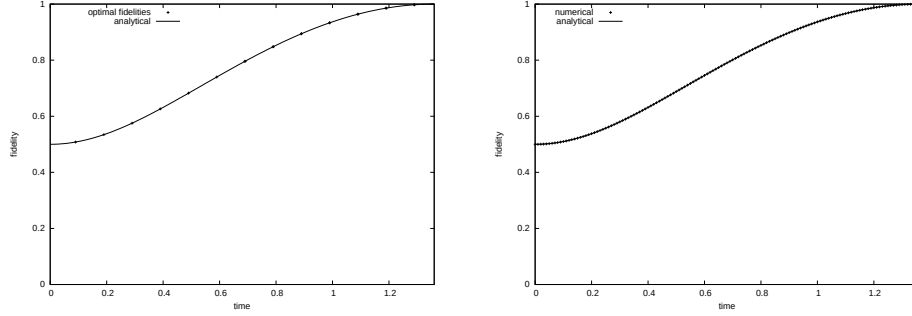


Figure 6.2: The left figure is the plot of optimal fidelities, derived by Krotov’s numerical method, for each duration time indicated by points and the time evolution of the fidelity derived in the section (4.3.1). The right figure is a comparison between the analytic solution and the numerical solution to generate the swap gate in the minimum time. The numerical solution plotted on the right figure reaches the point which has the fidelity to the target $f_{\text{num}}(t) = 1.0 - 1.3 \times 10^{-6}$ at $t = 1.36/\omega$, whereas the analytic solution is $f(T) = 1$ at $T = \frac{\sqrt{3}\pi}{4\omega} \simeq 1.360/\omega$.

In this case, the left figure 6.2 indicates that the optimal fidelity attainable in the fixed duration coincides with the time evolution of the fidelity along the time-optimal evolution toward the target.

6.6 Comparison with the simulated annealing method

To compare this Krotov method and the simulated annealing method, we compute the fidelity optimal evolution for the CNOT gate. The system is the two qubit model which is the same as that we used for the simulated annealing method

$$H = J\boldsymbol{\sigma}^1 \cdot \boldsymbol{\sigma}^2 + \mathbf{B}^1(t) \cdot \boldsymbol{\sigma}^1 + \mathbf{B}^2(t) \cdot \boldsymbol{\sigma}^2. \quad (6.64)$$

The constraint $|\mathbf{B}^1|^2 + |\mathbf{B}^2|^2 = \omega^2$ is imposed through the Lagrange multiplier $\gamma(t) = \sqrt{|\mathbf{B}^1(t)|^2 + |\mathbf{B}^2(t)|^2}/\omega$.

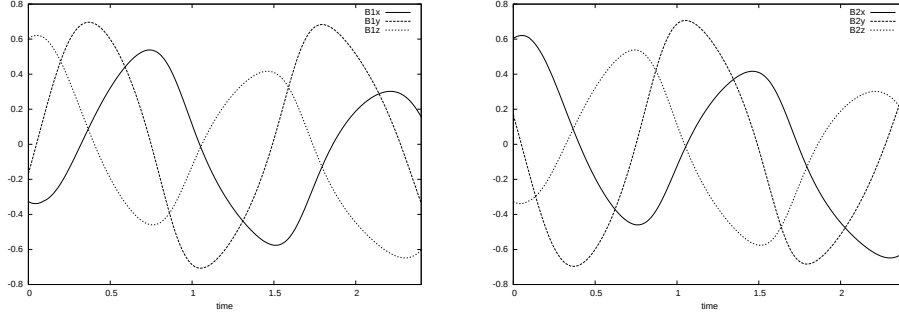


Figure 6.4: The optimal control for the external fields $\mathbf{B}_1(t)$ and $\mathbf{B}_2(t)$ for $T = 2.4$ case. Note that $B_x^1(t) = B_z^2(t)$, $B_y^1(t) = -B_y^2(t)$ and $B_z^1(t) = B_x^2(t)$, which means that the motion of $\mathbf{B}_1(t) + \mathbf{B}_2(t)$ is one-dimensional (see (5.15)).

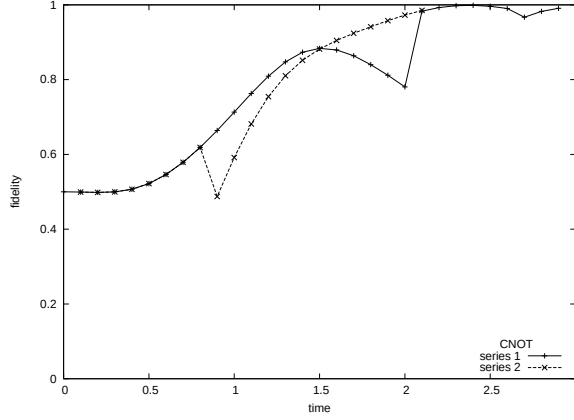


Figure 6.3: The relation between the time duration T and the optimal fidelity $f = \frac{1}{4} |\text{Tr} U_{\text{CNOT}}^\dagger U(T)|$. Each point is the result of Krotov's iteration for the unitary evolution from $U(0) = I$ to $U(T)$. There are two series of solutions chained by the output recycling. In a series, the connection indicates that the initial input field $\varepsilon^{(0)}$ for the next step is coming from the previous result. One series is starting from $T = 0.1$ to $T = 2.9$, the other is from $T = 2.1$ to $T = 0.1$. The maximum point in those series is $f = 0.998$ when the duration time is $T = 2.4$. From this plot, we can see that there are two continuous series of optimal evolutions and the front line is switched around $T = 1.5$.

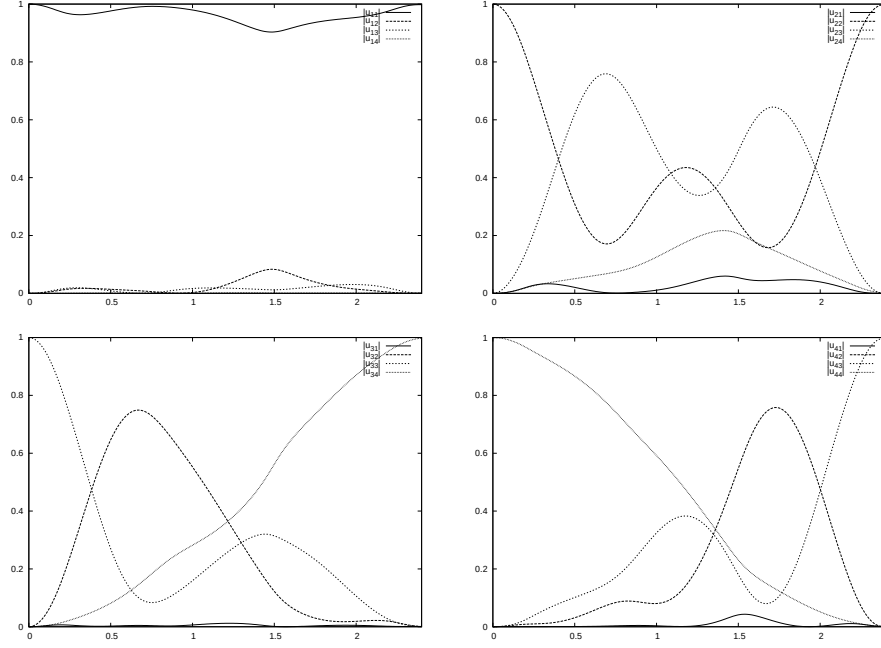


Figure 6.5: Time evolution of components of the unitary matrix.

In Chapter 5 we have analysed the same problem by the simulated annealing method. The numerical computations are performed for the same condition $J = 1.0$ and $\omega = 1.0$. The corresponding results are shown in the table 6.1, in which we can see the computational cost of the Krotov method is quite small compared to the simulated annealing method. Even there is no guarantee that we can get the optimal control which maximizes the cost functional by the Krotov method, the resultant control sequence is useful in practice, if it gives the control to get a desired unitary gate within a shorter time than the known “efficient” control.

	fidelity	duration time	iterations
Annealing	0.998	3.44	$\sim 10^5$
Krotov	0.996	2.4	$\sim 10^2$

Table 6.1: Results for the simulated annealing method and the Krotov method. The Krotov method is computed for the steps $T = 0.1 \times m$ ($m = 1, \dots, 29$) for the duration time. The iteration count is the order of the calculated full time evolution from $t = 0$ to $t = T$.

6.7 Comparison with the conventional method

There is an analytic way to make a controlled- U gate (see Appendix D). To make a comparison, we choose the same Hamiltonian

$$H = J\sigma_z^1\sigma_z^2 + \mathbf{B}^1 \cdot \boldsymbol{\sigma}^1 + \mathbf{B}^2 \cdot \boldsymbol{\sigma}^2. \quad (6.65)$$

We compute the fidelity optimization problem with the following constraint for several points in a range of time

$$\frac{1}{4} \text{Tr } H^2 = J(t)^2 + |\mathbf{B}^1(t)|^2 + |\mathbf{B}^2(t)|^2 = \omega^2 \quad (6.66)$$

where every coefficients are assumed to be controllable and ω is a constant. By reparametrizing time as the same way considered in the section 6.4.2, the coupling J can be regarded as a constant after the computation. The solutions for several duration times are derived (see figure 6.6).

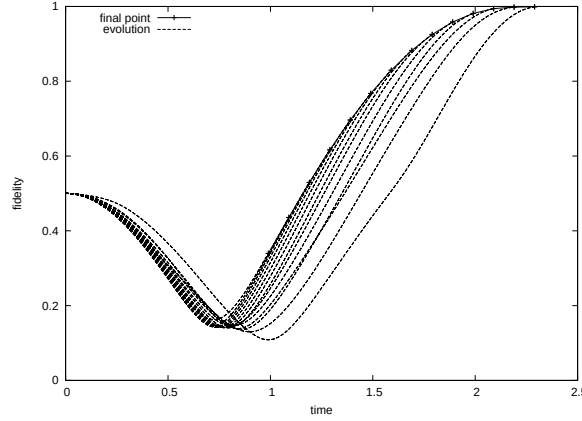


Figure 6.6: Each dotted curve corresponds to the time evolution of the fidelity in a fixed duration time in the range $T = 1.0/\omega$ to $T = 2.3/\omega$. Final points are the optimal fidelity which can be attained in the fixed time. The fidelity is converged around $T = 2.2/\omega$ which can be regarded as the optimal time to get the CNOT gate.

To generate the CNOT gate by the analytic way, the required time for the two-qubit interaction by the coupling Hamiltonian $H_0 = J\sigma_z^1\sigma_z^2$ is $\frac{\pi}{4J}$. The total time which contains the time cost for one-qubit operations measured

with the normalization condition for the Hamiltonian is $\frac{4\pi}{3\omega} \simeq 4.18/\omega$ (see Appendix D), whereas the result of the numerical computation is $2.3/\omega$.

6.8 Example: quantum Fourier transform

The quantum Fourier transform (QFT) is a key element of the quantum algorithms. The standard way to generate the QFT gate is to build from some elementary unitary gates. Instead, we make the whole QFT at once, which may decrease the duration time necessary for generating the target. The target is

$$U_{\text{QFT}} = \frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} \sum_{k=0}^{2^n-1} \exp \frac{2\pi i j k}{2^n} |j\rangle \langle k| \quad (6.67)$$

where $|j\rangle$ represents the n -qubit state in the binary representation (see Chapter 2).

We choose an n -qubit model with the Hamiltonian

$$H = \sum_{j=1}^{n-1} J_{j,j+1} \sigma_z^{(j)} \sigma_z^{(j+1)} + \sum_{j=1}^n \sum_{k=x,y,z} B_k^{(j)}(t) \sigma_k^{(j)} \quad (6.68)$$

where couplings $J_{j,j+1}$ are constants and $B_k^{(j)}(t)$ are assumed to be controllable. To seek the optimal control, we choose a constraint $J_{j,j+1} = 1.0$ and $|\mathbf{B}^1(t)|^2 + |\mathbf{B}^2(t)|^2 = 1.0$. To compare the conventional quantum circuit to realize n -qubit QFT gate from elemental gates and the one-step realization, we compute each duration time to obtain a elemental gate.

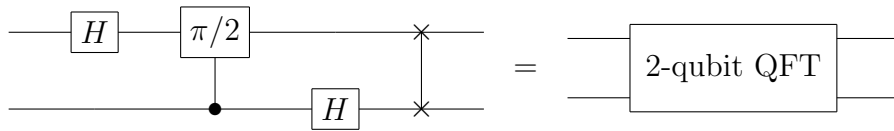


Figure 6.7: Two-qubit quantum Fourier transformation gate. H indicates the Hadamard gate, $\frac{\pi}{2}$ with a connection is the controlled phase gate and the two crosses with a connection is the swap gate.

As the result of numerical computation, we get tables 6.2, 6.3 and 6.4 for two-, three- and four-qubit QFT, respectively.

	H	$\pi/2$	SWAP	2-qubit QFT
time	2.5	3.3	3.8	3.2

Table 6.2: The duration time to realize corresponding gates within fidelity range larger than 0.997. The magnitude of external fields and the coupling is fixed to be $|\mathbf{B}^{(1)}|^2 + |\mathbf{B}^{(2)}|^2 = J = 1.0$. Ordinary cascading gates requires longer duration time than one step realization.

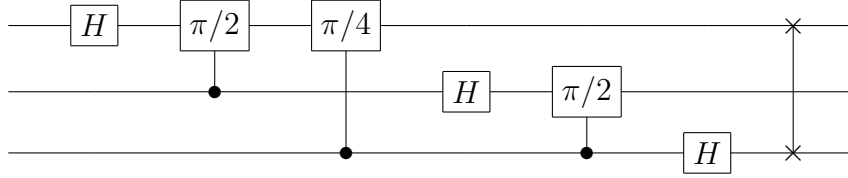


Figure 6.8: The quantum circuit for the three-qubit QFT.

	H	$\pi/2$	$\pi/4$	SWAP	3-qubit QFT
time	1.7	2.4	3.2	6.5	5.7

Table 6.3: The duration time to realize each elemental gates and the three-qubit QFT within fidelity range larger than 0.97.

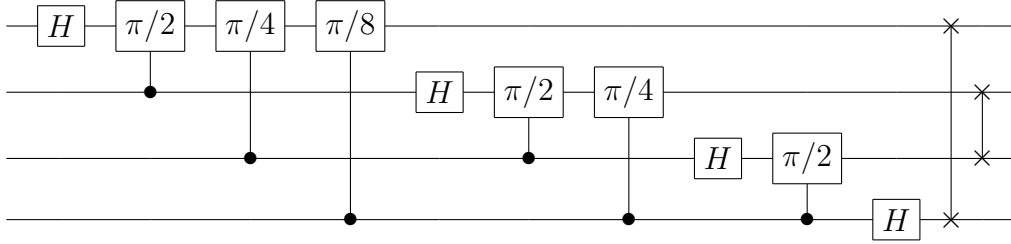


Figure 6.9: The quantum circuit for the four-qubit QFT.

	H	$\pi/2$	$\pi/4$	$\pi/8$	SWAP	4-qubit QFT
time	1.6	2.7	3.0	2.7	15	9.0

Table 6.4: The duration time to realize each elemental gate and the four-qubit QFT within fidelity range larger than 0.95.

For two-, three- and four-qubit QFT gate, we obtain the fidelity and time relation (see figure 6.10). The plot indicates that the required time to make the n -qubit QFT gate increases monotonically with the number of qubits n .

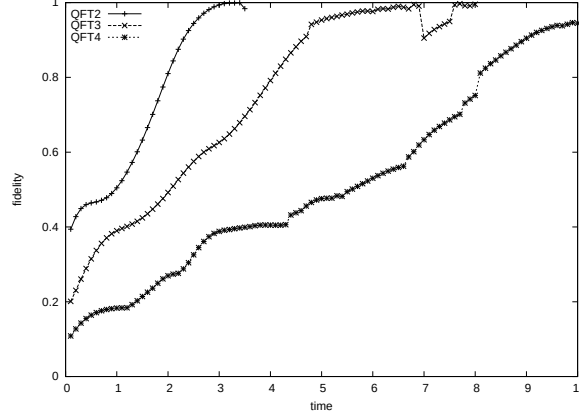


Figure 6.10: The relation between the time duration T and the optimal fidelity $f(U_{\text{QFT}}, U(T))$ for two-, three- and four-qubit models. The strength of couplings and magnitude of external fields are fixed to $J_{j,j+1} = 1$ and $\sum_j |\mathbf{B}^{(j)}|^2 = 1$.

The minimum duration time to generate n -qubit QFT gate is considered in Appendix F.

The evolution of the fidelity of a unitary toward the two-qubit QFT gate is shown in the figure 6.11. We can see that the optimal control is given for each choice of the fidelity which we want to attain.

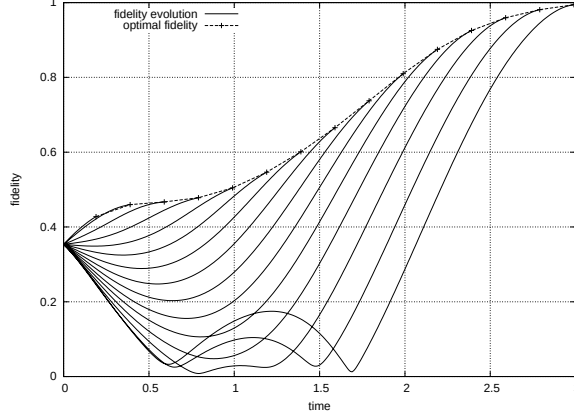


Figure 6.11: The solid curves are evolutions of the fidelity of a unitary toward the optimal fidelity. The dotted curve is the envelope of the optimal fidelities.

6.9 Time evolution of the entanglement

It is pointed out that the entanglement enhances the speed of evolution [36, 37, 38, 39]. To see the behavior of the entanglement in the time-optimal evolution, we consider the evolution of state from $|\psi(0)\rangle = |0\rangle_1 \otimes |0\rangle_2$,

$$|\psi(t)\rangle = U(t) |\psi(0)\rangle. \quad (6.69)$$

The entanglement is evaluated by the von Neumann entropy S of the mixed state ρ which is given by the partial trace over the second qubit

$$\rho(t) = \text{Tr}_2[U(t) |\psi(0)\rangle \langle\psi(0)| U^\dagger(t)] \quad (6.70)$$

$$S(t) = -\text{Tr} \rho(t) \log \rho(t). \quad (6.71)$$

From the figure 6.12, we can see that the entanglement between two qubits has peaks in the evolution. The role of entropy in the quantum brachistochrone is an open question.

6.10 Summary

In this chapter, we have introduced the Krotov iteration method and modified to the unitary evolution. We have seen the way how to apply this method

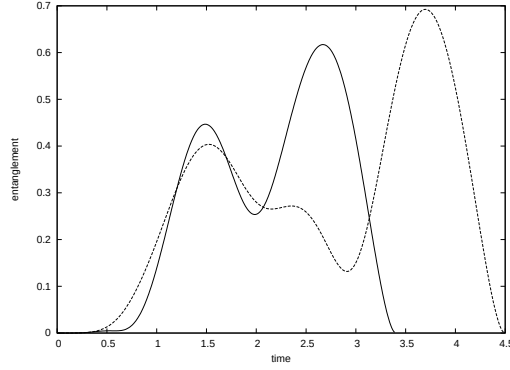


Figure 6.12: The behavior of entanglement for two trajectories obtained by the numerical method.

to the time-optimal control problem. By solving the fidelity optimization problem for many choice of duration times $T_1, T_2, \dots$, we obtain the relation between the fidelity to the target and the duration time. The required time to realize a unitary operation at a given fidelity range is obtained as a function of the fidelity and the corresponding control is derived for each T_i . To avoid the redundancy of the penalty approach, we have chosen a constraint for the controllable fields.

We have estimated the required time to make a multi-qubit unitary transformation by the conventional method realized by applying several elemental gate and a whole unitary transformation at once. It is confirmed that the required time for making at once is shorter. Also, we have seen the time-optimal generation of the quantum Fourier transform for a model for the n -qubit system.

Chapter 7

Ancilla assisted quantum evolution

Let us consider a system with an environment. The whole closed system is governed by the Schrödinger equation with a controllable Hamiltonian $H(t)$ and the evolution of the system can be obtained by

$$\rho(t) = \text{Tr}_E\{U(t)\rho(0) \otimes \rho_E U^\dagger(t)\}, \quad (7.1)$$

where ρ_E is the initial state of the environment and $U(t) = \mathcal{T} \exp(-i \int H(t)dt)$. Suppose we want to steer the state of the system from ρ_i to the target ρ_f regardless of the final state of the environment. If we know the Hamiltonian of the whole system, we can find the time-optimal unitary U_i which gives the state ρ_f , i.e. $\rho_f = \text{Tr}_E[U_i(T_i)\rho_i \otimes \rho_E U_i^\dagger(T_i)]$, where each $U_i(t)$ is given as a solution of the quantum brachistochrone and T_i is the corresponding duration time. The time-optimal evolution of the state of the system is found from the time-optimal evolutions in the whole system. Since there are many candidates for the evolutions $U_i(t)$ leading to ρ_f , we have to find the optimal one which has the minimum duration time T_i .

7.1 Two qubit model

In the section 4.3, we obtained the time-optimal unitary operator (4.50) for certain two-qubit system. Let us regard the first qubit as a system and the second as an environment and suppose the initial state of the whole system is $\rho_{SE} = |\uparrow\rangle\langle\uparrow| \otimes \rho_E(0)$ where $\rho_E(0) = \frac{1}{2}(I + \mathbf{x} \cdot \boldsymbol{\sigma})$. The unitary evolution

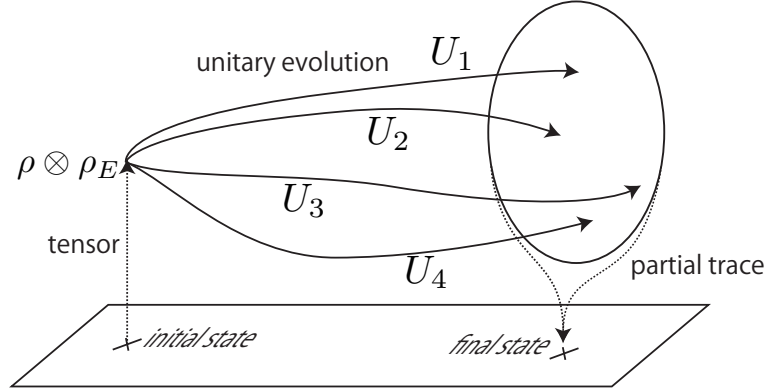


Figure 7.1: The parallelogram indicates the system and the circle indicates the range of the states which becomes the desired final state by the partial trace.

and the partial trace over the environment give the evolution for the system

$$\begin{aligned} \rho(t) &= \text{Tr}_E(U(t) |\uparrow\rangle \langle\uparrow| \otimes \rho_E(0) U^\dagger(t)) \\ &= \frac{1}{2} \left\{ \begin{aligned} &((\alpha_{0+}^2 + \alpha_{z+}^2)(1+z) + (\alpha_{0-}^2 + \alpha_{z-}^2)(1-z)) |\uparrow\rangle \langle\uparrow| \\ &+ \begin{pmatrix} e^{2iJ_3t}(\alpha_{0+} + i\alpha_{z+})(-\alpha_{y-} - i\alpha_{x-})(x - iy) \\ + e^{-2iJ_3t}(\alpha_{0-} + i\alpha_{z-})(-\alpha_{y+} - i\alpha_{x+})(x + iy) \end{pmatrix} |\uparrow\rangle \langle\downarrow| \\ &+ \begin{pmatrix} e^{-2iJ_3t}(\alpha_{0+} - i\alpha_{z+})(-\alpha_{y-} + i\alpha_{x-})(x + iy) \\ + e^{2iJ_3t}(\alpha_{0-} - i\alpha_{z-})(-\alpha_{y+} + i\alpha_{x+})(x - iy) \end{pmatrix} |\downarrow\rangle \langle\uparrow| \\ &+ ((\alpha_{x-}^2 + \alpha_{y-}^2)(1-z) + (\alpha_{x+}^2 + \alpha_{y+}^2)(1+z)) |\downarrow\rangle \langle\downarrow| \end{aligned} \right\}. \end{aligned} \quad (7.2)$$

If the initial state of the environment is $\rho_E(0) = |\uparrow\rangle \langle\uparrow|$, we have $x = y = 0, z = 1$ and

$$\rho(t) = \begin{bmatrix} \alpha_{0+}^2 + \alpha_{z+}^2 & 0 \\ 0 & \alpha_{x+}^2 + \alpha_{y+}^2 \end{bmatrix}. \quad (7.4)$$

The condition $\gamma_+ = 0$ and $\cos 2\psi_+ = 0$ yields

$$\rho(t) = \begin{bmatrix} \cos^2 B_{0+}t & 0 \\ 0 & \sin^2 B_{0+}t \end{bmatrix}. \quad (7.5)$$

The fastest transition from $|\uparrow\rangle$ to $|\downarrow\rangle$ can be given by choosing $B_{0+} = \sqrt{2}\omega, B_{0-} = 0$ and $J_3 = 0$, namely $H = \pm \frac{\omega}{\sqrt{2}}(\sigma_x \otimes \sigma_x - \sigma_y \otimes \sigma_y)$. The duration time is $T = \frac{\pi}{2\sqrt{2}\omega}$.

On the other hand, if the environment is completely mixed $\rho_E = \frac{1}{2}I$, we have

$$\rho(t) = \begin{bmatrix} \alpha_{0+}^2 + \alpha_{z+}^2 + \alpha_{0-}^2 + \alpha_{z-}^2 & 0 \\ 0 & \alpha_{x-}^2 + \alpha_{y-}^2 + \alpha_{x+}^2 + \alpha_{y+}^2 \end{bmatrix}. \quad (7.6)$$

By choosing $\gamma_{\pm} = 0$ and $\cos 2\psi_{\pm} = 0$, we obtain

$$\rho(t) = \frac{1}{2} \begin{bmatrix} \cos^2 B_{0+}t + \cos^2 B_{0-}t & 0 \\ 0 & \sin^2 B_{0+}t + \sin^2 B_{0-}t \end{bmatrix}. \quad (7.7)$$

The optimal choice for the transition $|\uparrow\rangle$ to $|\downarrow\rangle$ is $J_3 = 0$ and $B_{0+} = B_{0-} = \omega$, namely $H = \pm\omega\sigma_x \otimes \sigma_x$ or $H = \pm\omega\sigma_y \otimes \sigma_y$. The corresponding duration time is $T = \frac{\pi}{2\omega}$. This indicates that without the knowledge of the state of environment, we cannot make transitions faster.

Chapter 8

Quantum brachistochrone for mixed states

In this chapter, we consider the time-optimal control for open quantum systems where the state is governed by the master equation in the Lindblad form

$$\dot{\rho} = \mathcal{L}(\rho) = -i[H, \rho] + \sum_a (L_a \rho L_a^\dagger - \frac{1}{2} \{L_a^\dagger L_a, \rho\}) \quad (8.1)$$

where ρ is the density operator and H is the Hamiltonian, L_a ($a = 1, \dots, N^2-1$) are the Lindblad operators, N is the dimension of the Hilbert space of the system and we use the notation $\{A, B\} = AB + BA$ for the anti-commutator. We assume that a certain part of the Hamiltonian and the Lindblad operators are controllable.

8.1 Master equation

The meaning of the master equation can be seen by introducing an environment which is interacting with the system:

$$H = H_S \otimes I + H_{\text{int}}. \quad (8.2)$$

The time evolution of the state governed by the Lindblad form of the master equation comes from the repetition of the unitary evolution by the interaction

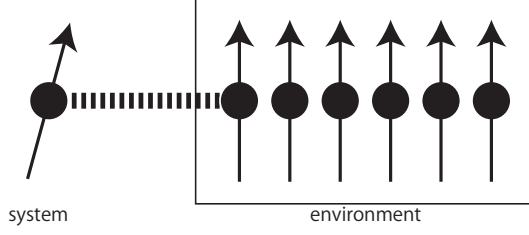


Figure 8.1: The system is interacting with the environment.

H_{int} for a short time duration ε , see e.g.[42], namely

$$\begin{aligned}
 \rho(t + \varepsilon) &= \text{Tr}_E[e^{-iH\varepsilon}\rho(t) \otimes \rho_E(t)e^{iH\varepsilon}] \\
 &= \rho(t) - i\varepsilon \text{Tr}_E[H, \rho(t) \otimes \rho_E(t)] \\
 &+ \varepsilon^2 \left\{ \text{Tr}_E[H\rho(t) \otimes \rho_E(t)H] - \frac{1}{2} \text{Tr}_E\{H^2, \rho(t) \otimes \rho_E(t)\} \right\} \\
 &+ \mathcal{O}(\varepsilon^3).
 \end{aligned} \tag{8.3}$$

For simplicity, we can restrict the Hamiltonian to be traceless without loss of generality. The traceless $N \times N$ Hermitian matrices A can be expanded in terms of orthonormal basis $\{F_i\}$ ¹ as $A = \sum_i F_i \frac{1}{N} \text{Tr}[AF_i]$. The operators acting on the composite system $\mathcal{H} \otimes \mathcal{H}_E$ is similarly expanded by basis $E_i \otimes I, E_i \otimes F_j$ and $I \otimes F_j$, ($i = 1, \dots, N^2 - 1$, $j = 1, \dots, N_E^2 - 1$), where we assume the dimension of the Hilbert space for the system and the environment is N and N_E , respectively. The interaction Hamiltonian acting on $\mathcal{H} \otimes \mathcal{H}_E$ is also expanded as

$$H_{\text{int}} = \sum_{i=1}^{N^2-1} \sum_{j=1}^{N_E^2-1} h_{ij} E_i \otimes F_j. \tag{8.5}$$

The equation (8.4) can be written as

$$\rho(t + \varepsilon) = \rho(t) - i\varepsilon[\tilde{H}(t), \rho(t)] + \sum_{ij} \varepsilon^2 a_{ij} (E_i \rho(t) E_j - \frac{1}{2} \{E_j E_i, \rho(t)\}) \tag{8.6}$$

where

$$\tilde{H}(t) = H_S + \sum_{ij} h_{ij} E_i \text{Tr}[F_j \rho_E(t)] \tag{8.7}$$

$$a_{ij}(t) = \sum_{kl} h_{ik} h_{jl} \text{Tr}[F_k \rho_E(t) F_l]. \tag{8.8}$$

¹It is orthonormalized on the Hilbert-Schmidt inner product $\text{Tr} F_i F_j = N \delta_{ij}$.

Since a_{ij} is a Hermitian matrix, it can be diagonalized by a unitary matrix u as $a_{ij} = \sum_k u_{ik} u_{jk}^* \gamma_k$. Introducing a set of operators $L_k = \sum_i E_i u_{ik} \sqrt{\gamma_k}$ which are called Lindblad operators, one can rewrite (8.6) as follows

$$\frac{d\rho}{dt} = \mathcal{L}(\rho) = -i[\tilde{H}, \rho] + \sum_i (L_i \rho L_i^\dagger - \frac{1}{2} \{L_i^\dagger L_i, \rho\}) \quad (8.9)$$

which is known as the Lindblad form of the master equation.

8.2 Invariance of the master equation

The evolution of $\rho(t)$ described by the master equation (8.1) is invariant under the following gauge transformations [42, p119],

$$\begin{aligned} H &\mapsto H + \alpha(t)I + \frac{1}{2i} \sum_a [\beta_a^*(t) L_a - \beta_a(t) L_a^\dagger], \\ L_a &\mapsto L_a + \beta_a(t)I, \end{aligned} \quad (8.10)$$

and

$$H \mapsto H, \quad L_a \mapsto \sum_b U_{ab}(t) L_b, \quad (8.11)$$

where $\alpha(t)$ is real, $\beta_a(t)$ are complex, and $U_{ab}(t)$ form a unitary matrix with respect to its indices (i.e., $\sum_c U_{ac} U_{bc}^* = \sum_c U_{ca}^* U_{cb} = \delta_{ab}$). The parameter $\alpha(t)$ in (8.10) corresponds to the $U(1)$ gauge degree of freedom. The gauge degrees of freedom $\beta_a(t)$, instead, correspond to the fact that the operator $H(t)$ in (8.1) is not just the free Hamiltonian of the reduced system, but may contain coupling terms with the environment (see, e.g., (8.7)). Finally, the $U_{ab}(t)$ represent the freedom of the choice of the basis for the Hilbert space of the environment. From this gauge freedom of the master equation (8.1), we can always choose H and L_a to be traceless and also L_a to be mutually orthogonal. In the following, we choose this gauge choice.

8.3 Optimal control problem

Let us consider the time-optimization problem for the open quantum system governed by the Lindblad form of the master equation. We assume that a

certain part of the Hamiltonian and the Lindblad operators can be controlled depending on the system, and constraints for the Hamiltonian and the Lindblad operators are independent. According to the scheme of the quantum brachistochrone discussed in the section 3.2 or 3.4, we consider the following action for mixed states evolution

$$S = \int_0^1 d\tau \left(\alpha + \text{Tr} \left[\sigma \left(\frac{d}{d\tau} \rho - \alpha \mathcal{L}(\rho) \right) \right] + L_C \right) \quad (8.12)$$

where the third term consists of constraints for the Hamiltonian and the Lindblad operators,

$$L_C = \sum_m \bar{\lambda}_m f_m(H) + \sum_{ab} \bar{\mu}_{ab} [\text{Tr} L_a^\dagger L_b - N \gamma_a^2 \delta_{ab}]. \quad (8.13)$$

In this constraint (8.13), the real functions $\bar{\lambda}_m$ and the Hermitian matrix $\bar{\mu}_{ab} = \bar{\mu}_{ba}^*$ ² are Lagrange multipliers to impose constraints

$$f_m(H) = 0 \quad (8.14)$$

on the Hamiltonian and orthogonality condition

$$\text{Tr} L_a^\dagger L_b = N \gamma_a \delta_{ab}. \quad (8.15)$$

on the Lindblad operators, respectively. In the second term of (8.12), σ is a Lagrange multiplier which gives the master equation

$$\frac{d}{d\tau} \rho = \alpha \mathcal{L}(\rho). \quad (8.16)$$

The first term $\int_0^1 \alpha d\tau$ gives the duration time by obtaining the time scale from the second term. By taking a variation with respect to α , we have

$$\text{Tr} \sigma \mathcal{L}(\rho) = 1. \quad (8.17)$$

The variation with respect to ρ gives

$$\frac{d}{d\tau} \sigma = \text{traceless part of } [-\alpha \mathcal{L}^\dagger(\sigma)], \quad (8.18)$$

²The complex matrix $\bar{\mu}_{ab}$ is an Hermitian because the condition (8.15) is Hermite as a complex matrix with indices a and b .

where the operator $\mathcal{L}^\dagger$ is defined by $\text{Tr}[A^\dagger \mathcal{L}(B)] = \text{Tr}[\mathcal{L}^\dagger(A)B]$ ³, because the trace part of ρ is not a variable. The variation with respect to $L_a^\dagger$ yields

$$\text{traceless part of } [\sigma L_a \rho - \frac{1}{2} L_a \{\rho, \sigma\}] = \sum_b \mu_{ab} L_b \quad (8.19)$$

where $\mu_{ab} = \bar{\mu}_{ab}/\alpha$. To see the anti-symmetric part of the Hilbert-Schmidt inner product of $L_a^\dagger$ and the equation (8.19)

$$\text{Tr}[(\sigma L_b \rho - \frac{1}{2} L_b \{\rho, \sigma\}) L_a^\dagger - L_b (\sigma L_a \rho - \frac{1}{2} L_a \{\rho, \sigma\})^\dagger] = N \mu_{ba} \gamma_a^2 - N \mu_{ab}^* \gamma_b^2 \quad (8.20)$$

which is identical to

$$0 = N \mu_{ab} (\gamma_a^2 - \gamma_b^2) \quad (8.21)$$

because of the orthogonality condition (8.15) and the hermiticity of μ_{ab} , we can conclude that $\mu_{ab} = \delta_{ab} \mu_a$. Therefore, the relation (8.22) can be written

$$\text{traceless part of } [\sigma L_a \rho - \frac{1}{2} L_a \{\rho, \sigma\}] = \mu_a L_a \quad (8.22)$$

which is an eigenvalue equation with eigenvalues μ_a and the eigenvectors L_a . The variation with respect to the Hamiltonian H gives

$$F = -i[\rho, \sigma], \quad (8.23)$$

$$\text{where } F = \frac{\partial L_C}{\partial H} = \sum_m \lambda_m \frac{\partial f_m(H)}{\partial H}. \quad (8.24)$$

Taking the time derivative of (8.23) and using (8.1), (8.18) and (8.22), we obtain the quantum brachistochrone equation

$$i\dot{F} = [H, F]. \quad (8.25)$$

8.4 A one-qubit example

Let us now discuss as an explicit example of our general formalism the simple case of a one-qubit model where the Hamiltonian is subject only to the normalization constraint

$$f_0(H) = \frac{1}{2}(\text{Tr } H^2 - 2\omega^2) = 0, \quad (8.26)$$

³The explicit form of $\mathcal{L}^\dagger$ is $\mathcal{L}^\dagger(A) = i[H, A] + \sum_a (L_a^\dagger A L_a - \frac{1}{2} \{L_a^\dagger L_a, A\})$, which is not traceless in general, whereas $\mathcal{L}(A)$ is traceless for all A .

where ω is a given constant. In this case $F = \lambda_0 H$ and the quantum brachistochrone equation (8.25) becomes trivial, giving $H = \text{const}$ and $\lambda_0 = \text{const}$ (see the section 4.1). Our problem then reduces to that of solving the master equation (8.1) and the adjoint master equation (8.18) together with the algebraic equations (8.23) and (8.22) for $\rho(t)$, $L_a(t)$ and $\sigma(t)$. In the Pauli basis $\{\sigma_x, \sigma_y, \sigma_z\}$ these can be rewritten as equations for three-dimensional vectors. Namely, if we parametrize the states as

$$\rho(t) = \frac{1}{2}[I + \mathbf{r}(t) \cdot \boldsymbol{\sigma}], \quad (8.27)$$

$$\sigma(t) = \mathbf{s}(t) \cdot \boldsymbol{\sigma}, \quad (8.28)$$

and the Hamiltonian and the Lindblad operators as

$$H = \mathbf{h} \cdot \boldsymbol{\sigma}, \quad (8.29)$$

$$L_a(t) = \mathbf{l}_a(t) \cdot \boldsymbol{\sigma}, \quad (8.30)$$

where $\mathbf{r}$, $\mathbf{s}$ and $\mathbf{h} \in \mathbb{R}^3$ and $\mathbf{l}_a \in \mathbb{C}^3$, the master equation (8.1) and the adjoint master equation (8.18) can be rewritten as

$$\dot{\mathbf{r}} = 2[\mathbf{h} \times \mathbf{r} + \sum_{\mathbf{l} \in \{\mathbf{l}_a\}} (\text{Re}((\mathbf{l} \cdot \mathbf{r})\mathbf{l}^*) - |\mathbf{l}|^2 \mathbf{r} + i\mathbf{l} \times \mathbf{l}^*)], \quad (8.31)$$

$$\dot{\mathbf{s}} = 2[\mathbf{h} \times \mathbf{s} - \sum_{\mathbf{l} \in \{\mathbf{l}_a\}} (\text{Re}((\mathbf{l} \cdot \mathbf{s})\mathbf{l}^*) - |\mathbf{l}|^2 \mathbf{s})]. \quad (8.32)$$

Moreover, the algebraic equations (8.23) and (8.22) read

$$\mathbf{r} \times \mathbf{s} = \lambda_0 \mathbf{h} = \text{const}. \quad (8.33)$$

and

$$K(\mathbf{r}, \mathbf{s})\mathbf{l}_a = \nu_a \mathbf{l}_a, \quad (8.34)$$

where $K(\mathbf{r}, \mathbf{s})$ is the self-adjoint matrix

$$K_{ij}(\mathbf{r}, \mathbf{s}) = r_i s_j + r_j s_i - 2i \sum_k \epsilon_{ijk} s_k \quad (8.35)$$

with $i, j = 1, 2, 3$ and $\nu_a = 2(\mathbf{r} \cdot \mathbf{s} + \mu_a)$ is a real number.

Because of the constraints (8.26) and (8.33), the components of the Hamiltonian $\mathbf{h}$ are given by

$$\mathbf{h} = \begin{cases} \pm \omega \frac{\mathbf{r} \times \mathbf{s}}{|\mathbf{r} \times \mathbf{s}|} & \text{if } \mathbf{r} \times \mathbf{s} \neq \mathbf{0}, \\ \omega \mathbf{n} & \text{if } \mathbf{r} \times \mathbf{s} = \mathbf{0}, \end{cases} \quad (8.36)$$

where $\mathbf{n}$ is an arbitrary unit vector. The components of the Lindblad operators $\mathbf{l}_a$ are determined as eigenvectors of the eigenvalue equation (8.34) with the constraints (8.15), i.e. $|\mathbf{l}_a| = \gamma_a$.

At a given instant, we parametrize $\mathbf{r}(t)$ and $\mathbf{s}(t)$ as

$$\mathbf{r}(t) = r \left(\cos \frac{\theta}{2} \mathbf{e}_3 + \sin \frac{\theta}{2} \mathbf{e}_1 \right), \quad (8.37)$$

$$\mathbf{s}(t) = s \left(\cos \frac{\theta}{2} \mathbf{e}_3 - \sin \frac{\theta}{2} \mathbf{e}_1 \right), \quad (8.38)$$

where $\{\mathbf{e}_1(t), \mathbf{e}_2(t), \mathbf{e}_3(t)\}$ are orthonormal vectors, so that $\mathbf{r} \cdot \mathbf{s} = rs \cos \theta$, with $r \in [0, 1]$, $s > 0$ and $\theta \in [0, \pi]$. We can then rewrite the matrix K in (8.35) as

$$(K_{ij}) = 2s \begin{bmatrix} -r \sin^2 \frac{\theta}{2} & -i \cos \frac{\theta}{2} & 0 \\ i \cos \frac{\theta}{2} & 0 & i \sin \frac{\theta}{2} \\ 0 & -i \sin \frac{\theta}{2} & r \cos^2 \frac{\theta}{2} \end{bmatrix}. \quad (8.39)$$

If the conserved vector satisfies $\mathbf{r} \times \mathbf{s} = \mathbf{0}$, we can see that $\theta = 0$ (i.e. $\mathbf{r} = r\mathbf{e}_3$), and the components of the Lindblad operators are given by (8.34) and (8.39) as the following eigenvectors $\mathbf{l}_a$ ($a = -, 0, +$)

$$\mathbf{l}_-(t) = \frac{\gamma_-}{\sqrt{2}}(\mathbf{e}_1 - i\mathbf{e}_2), \quad (8.40)$$

$$\mathbf{l}_0(t) = \gamma_3 \mathbf{e}_3. \quad (8.41)$$

$$\mathbf{l}_+(t) = \frac{\gamma_+}{\sqrt{2}}(\mathbf{e}_1 + i\mathbf{e}_2), \quad (8.42)$$

in the ascending order of the corresponding eigenvalues. To simplify the analysis, we can move to the interaction picture by the transformation $\rho = U_0 \rho U_0^\dagger = \frac{1}{2}(I + \mathbf{r} \cdot \boldsymbol{\sigma})$ with $U_0(t) = \mathcal{T} \exp(-i \int H(t) dt)$ ($\mathcal{T}$ is the time-ordered product), so that the master equation (8.31) becomes

$$\dot{\mathbf{r}} = -2[(\gamma_+^2 + \gamma_-^2)\mathbf{r} - (\gamma_+^2 - \gamma_-^2)\mathbf{e}_3], \quad (8.43)$$

which guarantees $\dot{\mathbf{e}}_3 = \mathbf{0}$. Therefore we obtain the following solution for the Bloch vector in the interaction picture

$$\tilde{\mathbf{r}}(t) = \left[\frac{\gamma_+^2 - \gamma_-^2}{\gamma_+^2 + \gamma_-^2} + \left(r'(0) - \frac{\gamma_+^2 - \gamma_-^2}{\gamma_+^2 + \gamma_-^2} \right) e^{-2(\gamma_+^2 + \gamma_-^2)t} \right] \mathbf{e}_3. \quad (8.44)$$

If the magnitudes of the Lindblad operators are equal i.e. $\gamma_+ = \gamma_-$, the state will irretrievably lose the coherence, but the coherence can be recovered when the magnitudes of the Lindblad operators are different. Note that in this particular case the L_0 operator, which corresponds to a projective measurement along $\mathbf{e}_3$, is not effective for the state evolution while the amplitude damping channels L_+, L_- play a significant role in (8.44). The case $\mathbf{h} = \mathbf{0}$ is depicted in Figure 8.2.

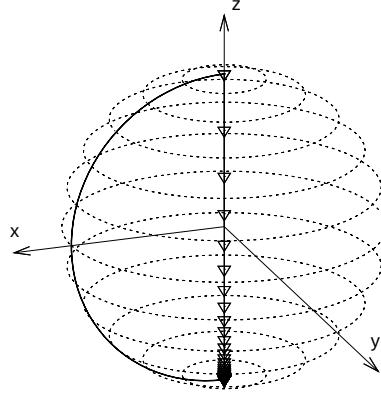


Figure 8.2: Analytical, time optimal evolution of $\rho(t)$ (arrows) in the Bloch sphere for the case of $\mathbf{r} \times \mathbf{s} = \mathbf{0}$, $\mathbf{r} \propto \mathbf{e}_z$, $\gamma_+ = 0$, $\gamma_- \neq 0$ and $\rho(0) = |\uparrow\rangle\langle\uparrow|$. Also shown (thick solid meridian curve) the optimal pure state evolution between the north and south poles.

In the case of $\mathbf{r} \times \mathbf{s} \neq 0$, the coupled equations (8.31), (8.32) and (8.34) are solved numerically. The eigenvectors are given by (8.34) for each instant, which will be non trivial when the determinant equals to zero:

$$f(\nu) = -\nu^3 + r \cos \theta \nu^2 + (1 + (\frac{r}{2})^2 \sin^2 \theta) \nu - r \cos \theta = 0 \quad (8.45)$$

whose solutions ν_j are eigenvalues of $K/2s$. It is easy to see from Figure 8.3

$$f(0) = -r \cos \theta \quad (8.46)$$

$$f(\pm 1) = \pm (\frac{r}{2})^2 \sin^2 \theta \quad (8.47)$$

$$f(\pm \infty) = \mp \infty \quad (8.48)$$

which indicates that the solution of (8.45) satisfies

$$(\nu_- = -1, \quad \nu_0 = r, \quad \nu_+ = 1 \quad \text{for } \theta = 0) \quad (8.49)$$

$$\nu_- < -1, 0 < \nu_0 < 1 < \nu_+ \quad \text{for } 0 < \theta < \frac{\pi}{2} \quad (8.50)$$

$$\nu_- = -1, \quad \nu_0 = 0, \quad \nu_+ = 1 \quad \text{for } \theta = \frac{\pi}{2} \quad (8.51)$$

$$\nu_- < -1 < \nu_0 < 0, 1 < \nu_+ \quad \text{for } \frac{\pi}{2} < \theta < \pi \quad (8.52)$$

$$(\nu_- = -1, \quad \nu_0 = -r, \quad \nu_+ = 1 \quad \text{for } \theta = \pi). \quad (8.53)$$

Thus eigenvalues will not cross each other during the continuous time evolution since the solution for $\theta = 0, \pi$ is in another branch. This fact justifies to interpret $\mathbf{l}_j(t + dt)$ as the continuous successor of $\mathbf{l}_j(t)$, to put suffix for them in the order of eigenvalues and to fix the amplitudes of them to be $|\mathbf{l}_j(t)| = \gamma_j$ in advance. We depict a family of optimal trajectories from a mixed state to a pure state in the Bloch sphere in Figure 8.4.

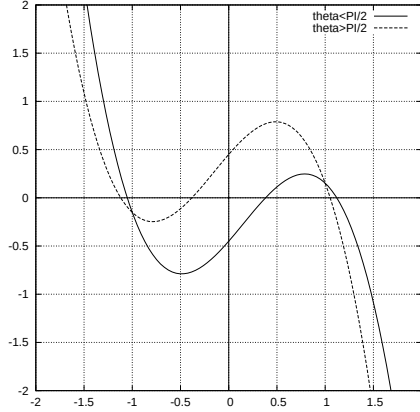


Figure 8.3: The determinant (8.45) as a function of ν . The solid curve is a typical shape of (8.45) for $0 < \theta < \frac{\pi}{2}$ and the dotted curve is for $\frac{\pi}{2} < \theta < \pi$.

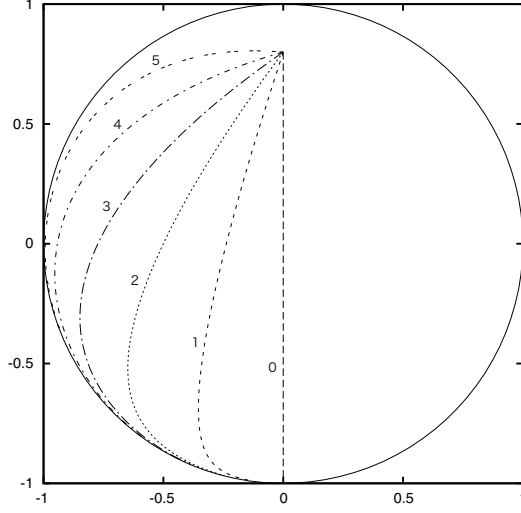
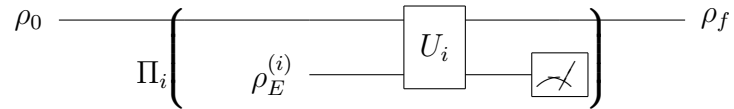


Figure 8.4: Time optimal evolutions of a mixed state governed by the master equation with the Lindblad operators having magnitudes $(\gamma_-, \gamma_0, \gamma_+) = (1, 0, 0)$ in the ascending order of the eigenvalues of (8.34), namely the only magnitude of the Lindblad operator corresponding to the minimum (negative) eigenvalue is nonzero. Curves starting from $\mathbf{r} = 0.8\mathbf{e}_z$ and approaching $\mathbf{r} = -\mathbf{e}_z$ are trajectories of the Bloch vector in the x - z plane cross-section of the Bloch sphere. The initial direction of the curves is different for each initial angle between $\mathbf{r}$ and $\mathbf{s}$, i.e. $\mathbf{r} \cdot \mathbf{s} = rs \cos \frac{n\pi}{6}$, $n = 0, 1, \dots, 5$.

8.5 A model for open system

In Section 8.1, we have seen that the mixed state evolution governed by the master equation in the Lindblad form is given by the repetition of the unitary evolution with external system E and the partial trace of E .



To get a further physical insight into our formalism, we study a simple model consisting of two interacting spins, one of which is identified with our system (S) and the other is an externally controllable ancilla (E). The ancilla system

E can be regarded as representing either a measurement apparatus or an environment. We choose two-qubit Hamiltonian as

$$H_{SE}(t) = \sum_{ij} h_{ij}(t) \sigma_i \otimes \sigma_j, \quad (8.54)$$

with time-dependent, tunable couplings $h_{ij}(t)$. We simulate the optimal Hamiltonian and Lindblad operators discussed in the previous section by tuning the couplings in (8.54) and the ancilla state. The state of the system is described by the density operator (8.27) and the state of the ancilla by

$$\rho_E(t) = \frac{1}{2}[1 + \mathbf{b}(t) \cdot \boldsymbol{\sigma}], \quad (8.55)$$

where $\mathbf{b}$ is a tunable Bloch vector. Using (8.7), we have

$$H(t) = \sum_{ij} h_{ij} b_j \sigma_i \quad (8.56)$$

$$a_{ij}(t) = \sum_{kl} h_{ik} h_{jl} \left(\delta_{kl} - i \sum_n \epsilon_{kln} b_n \right) \quad (8.57)$$

where the Pauli operators are used as the matrix basis.

The eigenvectors and the eigenvalues of (8.57) together define the components of the Lindblad operators. Therefore, since the same components are also the eigenvectors in (8.34), one has to impose the commutativity condition $[a, K] = 0$, where K is given by (8.35). The real and imaginary parts of the latter condition give three and nine constraints, respectively, so that we have twelve constraints in total for the nine parameters of h_{ij} and the three parameters of b_j . Then we can adjust the Hamiltonian couplings h_{ij} and the components b_j of the Bloch vector of the ancilla state so that the optimal $\mathbf{r}(t)$, $\mathbf{s}(t)$, $\mathbf{h}(t)$ and $\mathbf{l}_a(t)$ obtained in the previous section are reproduced.

In particular, if $\mathbf{r}$ and $\mathbf{s}$ are parallel (and chosen to be along the z -axis as at the end of the previous section), we can see that it is sufficient to choose the coupling matrix h_{ij} as

$$(h_{ij}) = \begin{bmatrix} 0 & p & 0 \\ p & 0 & 0 \\ 0 & 0 & q \end{bmatrix}, \quad (8.58)$$

with real numbers p, q , and the Bloch vector $\mathbf{b}$ as

$$\mathbf{b} = b \mathbf{e}_3. \quad (8.59)$$

The Hamiltonian and the Lindblad matrix (8.57) become, respectively,

$$H = qb\sigma_3 \quad (8.60)$$

$$(a_{ij}) = \begin{bmatrix} p^2 & ibp^2 & 0 \\ -ibp^2 & p^2 & 0 \\ 0 & 0 & q^2 \end{bmatrix}. \quad (8.61)$$

Then the K matrix (8.39) for $\theta = 0$,

$$(K_{ij}) = 2s \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & r \end{bmatrix}, \quad (8.62)$$

and the Lindblad matrix a_{ij} can be diagonalized simultaneously. In particular, the eigenvalues of a_{ij} are $p^2(1 \mp b)$, q^2 and the corresponding eigenvectors are given as in (8.40), (8.41) and (8.42), which leads to the Lindblad operators

$$L_{\pm} = \gamma_{\pm}\sigma_{\pm}, \quad (8.63)$$

$$L_0 = \gamma_0\sigma_3. \quad (8.64)$$

where $\gamma_{\pm}^2 = (1 \mp b)\tau p^2$, $\gamma_0^2 = \tau q^2$. The optimal solution for $\mathbf{r}(t)$ can be finally cast in the form

$$\mathbf{r}(t) = [-b + (r(0) + b)e^{-4p^2\tau t}]\mathbf{e}_3. \quad (8.65)$$

An intuitive explanation for the behavior of the Bloch vector is the following. The exponential damping in (8.65) can be attributed to the standard formula for the transition probability calculated from the interaction Hamiltonian defined by (8.58)

$$H_{SE} = p(\sigma_x \otimes \sigma_y + \sigma_y \otimes \sigma_x) + q\sigma_z \otimes \sigma_z. \quad (8.66)$$

Note that q does not appear in (8.65), because the optimal trajectory is $\mathbf{r}(t) \propto \mathbf{e}_3$, so that it can be put equal to zero. Suppose we have many qubits in the state $|\uparrow\rangle$, i.e. $b = 1$, as the environment that repeatedly interacts with the system. The interaction Hamiltonian (8.66) can be written

$$H_{SE} = 2ip(\sigma_+ \otimes \sigma_+ - \sigma_- \otimes \sigma_-), \quad (8.67)$$

which acts on the whole state $\rho(t) \otimes |\uparrow\rangle \langle\uparrow|$ repeatedly in a short duration, and gradually reduces the population of up spins while down spins unchanged. Even if the initial state is completely mixed state $r(0) = 0$, such a cooling process [43] works. The state of the system evolves from completely mixed state to a purely down state. On the other hand, if the environment is completely mixed, i.e. $b = 0$, the state approaches a completely mixed state.

Chapter 9

Summary and discussion

We have formulated the framework for time-optimal quantum control problems which we call the quantum brachistochrone. That is inspired by the brachistochrone problem and we have derived a universal equation: *quantum brachistochrone equation*

$$i\dot{F} = [H, F], \quad (9.1)$$

where the operator F comes from constraints for the system. This equation is valid for time-optimal control for pure state evolution from a given initial state to a desired final state $|\psi_i\rangle \rightarrow |\psi_f\rangle$, unitary operations from the identity operator to the target operator $I \rightarrow U$ and mixed state evolution $\rho_i \rightarrow \rho_f$. The unit of time is fixed by the magnitude of static term of the Hamiltonian or the constraint for the Hamiltonian. If there is a static term in the Hamiltonian, which is expressed by a constraint, the duration time is measured by the magnitude of it as a unit. On the other hand, if there are no static terms, we have to clarify what we optimize, because the time required to make an operation can be arbitrarily small by making the amplitude of Hamiltonian large. For this purpose, we have introduced a normalization condition for the N dimensional Hamiltonian $\text{Tr } H^2 = N\omega^2$ which clarifies the amount of available action per a unit of time. It is also possible to quantify the effect of Hamiltonian by using extra constraints or a cost function instead of (4.2) depending on the purpose which is related to the work by Nielsen *et al.* [44, 45, 46]. We have seen this relation in Appendix B.

The problem for the time-optimal unitary operations are formulated by a small modification from the time-optimal pure state evolution. It has greater relevance for quantum computation, since we need to prepare unitary operations as building blocks for the quantum computer regardless of initial states

which is unknown during a computation in general. We have solved the quantum brachistochrone problem for some models analytically, in which we have derived a general solution and fixed integration constants by equating the target and the solution up to phase. The optimal solution is found by choosing the set of constants which minimizes the duration time. This procedure needs messy calculations in practice even for a simple model composed by two qubits and there is no guarantee to be able to find the analytic solution. To avoid this analysis, we have introduced a simple numerical method based on the simulated annealing method in Chapter 5.

In Chapter 6, we have introduced the Krotov iteration method. By modifying this method, we have obtained a systematic and efficient way to solve the brachistochrone problem. The computational cost is surprisingly lower than the simulated annealing method. Using this method, we have confirmed that the required time to make a multi-qubit unitary transformation by the conventional method (realized by applying several elemental gates) is longer than the time necessary to perform a whole unitary transformation at once, provided that a common physical model is given. Also, we have seen that the optimal duration time, measured by the coupling constant, to generate the quantum Fourier transform for n -qubit system increases with the number of qubits.

We have considered two types of extensions for the time-optimal mixed state evolution. One is a composite quantum system discussed in Chapter 7, in which the evolution of a part of whole is optimized and the other part is thrown away (traced out). We have seen that we can make a transition of the system faster if we know the state of the ancilla. On the other hand, in Chapter 8, we have considered an extension of the quantum brachistochrone for the mixed state evolution governed by the master equation in the Lindblad form. The physical process behind of this formulation by the master equation, is the repeated interactions with the environment as a reservoir of states. The optimization was done for the abstract form of the master equation regardless of the physical realization. After that, we have considered a model which realize the optimal evolution of the mixed state derived by our formulation. In Figure 9.1 we plot the fidelity between the target pure state and the time optimal evolved mixed state as a function of the duration time of the evolution. We can see that, there is a domain that the fidelity of the mixed state evolution by the master equation is higher than the fidelity of the pure state evolution.

We have formulated the way to obtain time-optimal quantum evolutions,

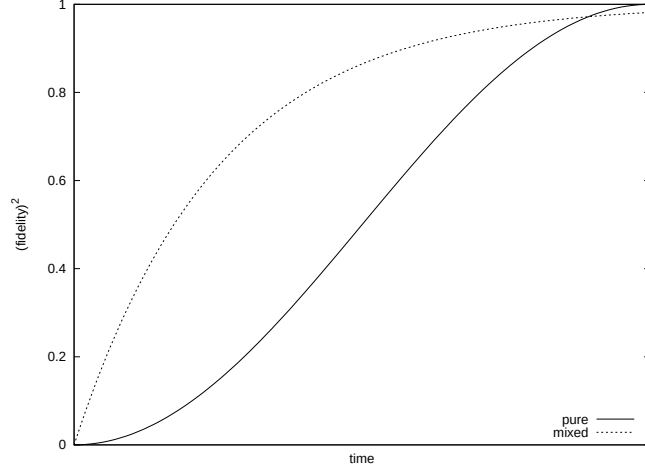


Figure 9.1: Time dependence of the fidelity squared $\langle \downarrow | \rho(t) | \downarrow \rangle$. The solid thick curve corresponds to the pure state evolution for a one-qubit system. The dashed curve corresponds to the repeated measurement case (8.65). Until the two curves cross each other, the repeated measurement model approaches the target $\rho_f = |\downarrow\rangle \langle \downarrow|$ faster than the pure state evolution.

what we call the quantum brachistochrone, and exemplified for several coherent and incoherent evolutions. Those particular analytical and numerical demonstrations suffice to shape a systematic methodology for quantum optimization problems, which can be applied to multi-qubit systems.

Acknowledgements

I am very grateful to Professor Akio Hosoya for continuous encouragement, kind advices and collaborations. I express my special thanks to Dr. Tatsuhiko Koike and Dr. Alberto Carlini for fruitful discussions and collaborations. I would like to express my thanks to all colleagues in Cosmology Group of Tokyo Institute of Technology to spend precious times for hearing my talks and giving me advices. I also thank Professor Seth Lloyd for providing me a chance to study at Massachusetts Institute of Technology and giving me suggestions and opinions. I would express my thanks to our secretaries for miscellaneous businesses to support our researches.

This work was supported by the 21st Century COE Program at Tokyo Institute of Technology “Nanometer-Scale Quantum Physics” by the Ministry of Education, Culture, Sports, Science and Technology of Japan.

Finally, I thank my family for their nonstop support.

Appendix A

Quantum speed limit

The speed of quantum computer is bounded by the duration time of the transition of quantum states. Anandan and Aharonov have shown an analytic bound on the required time for a transition from a state to the orthogonal state by using the Fubini-Study metric. Another quantum speed limit is found by Margolus and Levitin [26].

A.1 Fubini-Study metric

The Fubini-Study metric is obtained from the natural extension of the Fisher metric on the space of classical probability distributions to the space of quantum (pure) states, which can be seen as the infinitesimal angle between $|\psi\rangle$ and the neighbouring states $|\tilde{\psi}\rangle = |\psi\rangle + |d\psi\rangle$ in the Hilbert space as follows,

$$ds^2 = 4(\cos^{-1} |\langle \tilde{\psi} | \psi \rangle|)^2 \quad (\text{A.1})$$

$$= 4(1 - |\langle \tilde{\psi} | \psi \rangle|^2) \quad (\text{A.2})$$

$$= 4\langle d\psi_\perp | d\psi_\perp \rangle \quad (\text{A.3})$$

where we used the fact $|\langle \psi | \psi \rangle + \langle d\psi | \psi \rangle| = 1$ and defined $|d\psi_\perp\rangle = (1 - |\psi\rangle\langle\psi|)|d\psi\rangle$ in (A.3). The geodesic curve of the Fubini-Study metric is obtained with the gauge condition which is called a horizontal lift imposing the relation: $\langle \psi | \dot{\psi} \rangle = 0$ for the trace part of the Hamiltonian, as follows,

$$|\psi(s)\rangle = \cos(\omega s)|\psi(0)\rangle + \frac{\sin(\omega s)}{\omega}|\dot{\psi}(0)\rangle, \quad (\text{A.4})$$

where $\omega = \langle \dot{\psi} | \dot{\psi} \rangle^{1/2}$. The parameter which makes the state orthogonal to the initial state is $s_{\perp} = \frac{\pi}{2\omega}$. The quantum search algorithm found by Grover [5] is known to be optimal in which the quantum state passes through the geodesics (A.4) [47].

A.2 Anandan-Aharonov bound

The uncertainty relation of the energy and time has been revised by Anandan and Aharonov [25]. They have shown that the length measured by Fubini-Study metric $ds^2 = 4\langle d\psi | (1 - |\psi\rangle\langle\psi|) | d\psi \rangle$ is given by the standard deviation of the energy as follows

$$\Delta s = \int 2\langle \dot{\psi} | (1 - |\psi\rangle\langle\psi|) | \dot{\psi} \rangle^{1/2} dt \quad (\text{A.5})$$

$$= \int 2(\langle \dot{\psi} | H^2 | \dot{\psi} \rangle - \langle \dot{\psi} | H | \dot{\psi} \rangle^2)^{1/2} dt \quad (\text{A.6})$$

$$= \int 2\Delta E dt. \quad (\text{A.7})$$

Here we used the Schrödinger equation $i|\dot{\psi}\rangle = H(t)|\psi\rangle$. This equality gives the lower bound for the orthogonal time $t_{\perp}$, which is the time necessary to get distinct (orthogonal) state from an initial state. Since any paths between orthogonal states have length larger than π ,

$$t_{\perp} \geq \frac{\pi}{2\langle \Delta E \rangle} \quad (\text{A.8})$$

where $\langle \Delta E \rangle = \frac{1}{T} \int_0^T \Delta E dt$.

A.3 Margolus-Levitin bound

There is another quantum speed limit found by Margolus and Levitin [26]. They consider the minimum time for a transition between orthogonal states. Suppose we have an initial state $|\psi_0\rangle = \sum_n c_n |E_n\rangle$, where $|E_n\rangle$ are energy eigenstates of the system. Since the evolution is governed by the Schrödinger equation, the state will be

$$|\psi(t)\rangle = \sum_n c_n e^{-iE_n t} |E_n\rangle, \quad (\text{A.9})$$

where we take the origin of the energy and suffixes such that $0 = E_0 \leq E_1 \leq E_2 \leq \dots$. The real part of the inner product $\langle \psi_0 | \psi(t) \rangle$ can be written, by using the inequality $\cos x \leq 1 - \frac{2}{\pi}(x + \sin x)$ for any $x \geq 0$, as

$$\operatorname{Re} \langle \psi_0 | \psi(t) \rangle = \sum_n |c_n|^2 \cos(E_n t) \quad (\text{A.10})$$

$$\leq \sum_n |c_n|^2 \left(1 - \frac{2}{\pi}(E_n t + \sin(E_n t))\right) \quad (\text{A.11})$$

$$= 1 - \frac{2\langle E \rangle t}{\pi} + \frac{2}{\pi} \operatorname{Im} \langle \psi_0 | \psi(t) \rangle. \quad (\text{A.12})$$

When the state becomes orthogonal to the initial state, this inequality gives $0 \leq 1 - \frac{2\langle E \rangle t}{\pi}$, thus the lower bound of the orthogonal time is $t_\perp \geq \frac{\pi}{2\langle E \rangle}$, where the energy of the ground state E_0 is chosen to be the origin of the energy, or

$$t_\perp \geq \frac{\pi}{2(\langle E \rangle - E_0)} \quad (\text{A.13})$$

without energy shift.

A.4 Quantum speed limit

Since both of the limits for the orthogonal time $t_\perp$ shown above are valid, it is bounded by a longer one:

$$t_\perp \geq \max \left(\frac{\pi}{2(\langle E \rangle - E_0)}, \frac{\pi}{2\Delta E} \right). \quad (\text{A.14})$$

Giovannetti *et al.* [36] have generalized this bound as a function of the fidelity from the initial state. They bound the time for a transition of quantum states for a given Hamiltonian which is considered to be fixed.

Appendix B

Nielsen's geometric approach

Nielsen *et al.* derived a geodesic equation by defining the distance on the space of Hamiltonian [44, 45, 46]. In this appendix, we consider a relation of our method and their method. In their method, the distance is measured by the cost function

$$c(H) = \sqrt{\langle H, \mathcal{G}(H) \rangle} \quad (\text{B.1})$$

$$= \sqrt{\sum_{\sigma \in V} \text{Tr}^2(H\sigma) + p \sum_{\sigma \in \bar{V}} \text{Tr}^2(H\sigma)} \quad (\text{B.2})$$

where V is a set of generators whose coefficients in the Hamiltonian $\text{Tr}(H\sigma)$ can be controlled and $\bar{V}$ is the compliment whose coefficients are hard to control if a penalty parameter p is chosen to be large. The operator $\mathcal{G}$ in the cost function is defined as

$$\mathcal{G}(H) = \frac{1}{2^n} \left\{ \sum_{\sigma \in V} \text{Tr}(H\sigma)\sigma + p \sum_{\sigma \in \bar{V}} \text{Tr}(H\sigma)\sigma \right\}. \quad (\text{B.3})$$

They implement the Schrödinger evolution to make an unitary operator by introducing the Pauli coordinate, whereas we ensure it by the constraint. By taking variation of the total cost $\int c(H)dt$ with respect to the trajectory, one obtain a geodesic equation

$$i\dot{L} = [H, L] \quad (\text{B.4})$$

where $L = \mathcal{G}(H)$. If one choose $\bar{V}$ to be empty (or $p = 1$), (B.3) will be $\mathcal{G}(H) = \frac{1}{2^n} \text{Tr} H^2$ which corresponds to the case for choosing only one constraint $f_0(H) = \frac{1}{2}(\text{Tr} H^2 - 2^n \omega^2) = 0$ in our method. The solution for

the case with the penalty factor $p \rightarrow \infty$ for $\bar{V} = \sigma_z$ corresponds to our method with the additional constraint $f_1(H) = \text{Tr}(H\sigma_z) = 0$, for example. As we have considered in Chapter 4, to evaluate the time duration with the constraint $\frac{1}{2^n} \text{Tr} H^2 = \omega^2$ is equivalent to evaluate $\sqrt{\frac{1}{2^n} \text{Tr} H^2(t)}$ along the time evolution in a fixed duration time.

To clarify this similarity, we consider the intermediate action between our method and Nielsen's method,

$$S = \int_0^T dt \left\{ \text{Tr}(H\mathcal{G}(H)) + 2 \text{Re} \text{Tr}[V^\dagger(i\dot{U} - HU)] \right\} \quad (\text{B.5})$$

where V is a Lagrange multiplier to impose that the unitary operator governed by the Schrödinger equation. The variation with respect to H gives

$$\mathcal{G}(H) = UV^\dagger + VU^\dagger. \quad (\text{B.6})$$

Since U and V are governed by the Schrödinger equation, we obtain the geodesic equation (B.4) again. As the result, their approach is equivalent to consider the action (B.5). From the orthogonality of σ , the component parallels to $\sigma \in \bar{V}$ of (B.6) satisfies

$$\text{Tr}(H\sigma) = \frac{2}{p} \text{Re} \text{Tr}(V^\dagger \sigma U) \quad (\text{B.7})$$

which implies $\text{Tr}(H\sigma) \rightarrow 0$ when one choose $p \rightarrow \infty$. Thus we can realize the condition $\text{Tr}(H\sigma) = 0$ by choosing a large penalty factor instead of imposing the constraint. The difference between the intermediate action (B.5) and our action (3.25) is the way to impose constraint.

Appendix C

Quantum dots

A few electrons confined in semiconductor quantum dots are a candidate for the quantum computing device. There are some ways to implement qubit using quantum dots [40, 41]. We consider the time-optimal control for a simple implementation. One can use two charge states, in which an electron is confined in the left dot $|L\rangle$ or in the right dot $|R\rangle$. The effective Hamiltonian for this model [40] is simply

$$H(t) = \delta\sigma_x + \varepsilon(t)\sigma_z, \quad (\text{C.1})$$

where ε can be controlled by voltages of electrodes in the range $|\varepsilon| \leq \varepsilon_{\max}$. The constraints can be explicitly written as

$$f_1 = \text{Tr } H\sigma_x - 2\delta = 0, \quad (\text{C.2})$$

$$f_2 = \text{Tr } H\sigma_y = 0, \quad (\text{C.3})$$

$$f_3 = \left(\frac{1}{2} \text{Tr } H\sigma_z\right)^2 + \zeta^2 - \varepsilon_{\max}^2 = 0, \quad (\text{C.4})$$

where $f_1 = 0$ and $f_2 = 0$ fix the static part of the Hamiltonian, and ζ in f_3 is an auxiliary parameter ensuring $\varepsilon = \frac{1}{2} \text{Tr } H\sigma_z$ to be in the range. The operator F for this system is given by

$$F = \xi \frac{\partial f_1}{\partial H} + \eta \frac{\partial f_2}{\partial H} + \lambda \frac{\partial f_3}{\partial H} = \xi\sigma_x + \eta\sigma_y + \lambda\varepsilon\sigma_z \quad (\text{C.5})$$

where λ, ξ and η are the Lagrange multipliers. Taking variations with respect to λ and ζ , we have

$$\varepsilon^2 + \zeta^2 = \varepsilon_{\max}^2 \quad (\text{C.6})$$

$$\lambda\zeta = 0. \quad (\text{C.7})$$

The quantum brachistochrone equation $i\dot{F} = [H, F]$ gives following equations

$$\frac{d}{dt}(\lambda\varepsilon) = 2\eta\delta \quad (\text{C.8})$$

$$\frac{d}{dt}\xi = -2\varepsilon\eta \quad (\text{C.9})$$

$$\frac{d}{dt}\eta = 2\varepsilon(\xi - \lambda\delta), \quad (\text{C.10})$$

in which there is a constant

$$\xi^2 + \eta^2 + (\varepsilon\lambda)^2 = \text{constant}. \quad (\text{C.11})$$

We assume that the optimal control for $\varepsilon(t)$ consists of continuous segments and finite discontinuity. If there is a segment where $\lambda \neq 0$, we have $\zeta = 0$ from (C.7) and $|\varepsilon| = \varepsilon_{\max}$ from (C.6). Moreover, if there is another segment where $\lambda = 0$ in the same sequence, we have $\eta = 0$ and $\xi = \text{const.} \neq 0$ from (C.8), (C.9) and (C.11), and then $\varepsilon = 0$. Therefore, the pulse sequence

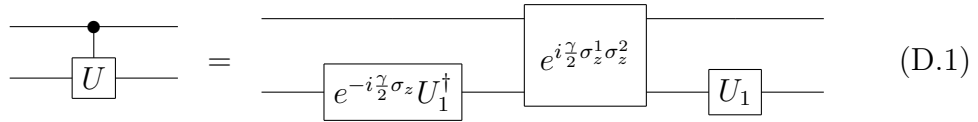
$$\varepsilon = \begin{cases} \pm\varepsilon_{\max} \\ 0 \end{cases} \quad (\text{C.12})$$

is obtained as a solution of the quantum brachistochrone, which means that the conventional control method supposed in e.g. [40] can be regarded as a time-optimal control.

Appendix D

Construction of two-qubit gate with impulsive local operations

The non-local two-qubit operations by using the static two-qubit coupling and the impulsive one-qubit operations are considered by many people, e.g [18, 19], in which the duration time to make local operations are assumed to be negligible. According to the proposition in the paper by Zhang *et al.* [20] the controlled- U gate can be constructed by the one-qubit local operation and the two-qubit interaction



$$\text{Controlled-}U = \text{[Circuit with } e^{-i\frac{\gamma}{2}\sigma_z U_1^\dagger}, e^{i\frac{\gamma}{2}\sigma_z^1 \sigma_z^2}, \text{ and } U_1 \text{]} \quad (\text{D.1})$$

where $U = \exp\{i\gamma \mathbf{n} \cdot \boldsymbol{\sigma}\}$ with a unit vector $\mathbf{n} = (n_x, n_y, n_z)$. The operator U_1 is defined as

$$U_1 = \begin{cases} \begin{bmatrix} i\sqrt{\frac{1-n_z}{2}} & \sqrt{\frac{1+n_z}{2}} \\ \frac{n_y - n_x i}{\sqrt{2(1-n_z)}} & \frac{n_x + n_y i}{\sqrt{2(1+n_z)}} \end{bmatrix} & \text{for } n_z \neq \pm 1, \\ \sigma_x & \text{for } n_z = 1, \\ I & \text{for } n_z = -1. \end{cases} \quad (\text{D.2})$$

To make a CNOT gate, the constants are chosen to be $\mathbf{n} = (1, 0, 0)$ and $\gamma = \frac{\pi}{2}$, namely $U = i\sigma_x$. The gate is decomposed into the following local gates and

the two qubit gate

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} = (U_2 \otimes I)(I \otimes U_1)e^{i\frac{\pi}{4}\sigma_z^1\sigma_z^2}(I \otimes U_1'), \quad (\text{D.3})$$

where $U_2 \otimes I$ removes an unwanted phase and these matrices are written with $\beta = e^{i\frac{\pi}{4}}$

$$U_1' = e^{-i\frac{\pi}{4}\sigma_z}U_1^\dagger = \frac{1}{\sqrt{2}} \begin{bmatrix} \beta^{-3} & \beta^1 \\ \beta^1 & \beta^1 \end{bmatrix} \quad (\text{D.4})$$

$$U_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} \beta^2 & \beta^0 \\ \beta^{-2} & \beta^0 \end{bmatrix} \quad (\text{D.5})$$

$$U_2 = \begin{bmatrix} \beta^0 & 0 \\ 0 & \beta^{-2} \end{bmatrix}. \quad (\text{D.6})$$

Each local operation U_k is performed by the local Hamiltonian $H_k = \mathbf{B} \cdot \boldsymbol{\sigma}$ up to a phase χ

$$U_k = e^{i\chi} \exp[-i\tau \mathbf{B} \cdot \boldsymbol{\sigma}], \quad (\text{D.7})$$

where τ is usually assumed to be small compared to the duration time of two-qubit interaction γ , in other words the magnitude of $\mathbf{B}$ is assumed to be large. To compare the duration time derived with the normalization constraint $\frac{1}{4} \text{Tr} H^2 = \omega^2$ for two qubit system in Section 6.7, we quantify the amount of applied field by $\sqrt{\frac{1}{4} \text{Tr}(H\tau)^2}$. The local gates (D.4), (D.5) and (D.6) are explicitly written as

$$I \otimes U_1' = e^{-i\frac{\pi}{4}} \exp\{i\frac{\pi}{2}I \otimes (\frac{1}{\sqrt{2}}\sigma_x - \frac{1}{\sqrt{2}}\sigma_y)\} \quad (\text{D.8})$$

$$I \otimes U_1 = e^{-i\frac{3\pi}{4}} \exp\{i\frac{\pi}{3}I \otimes (-\frac{1}{\sqrt{3}}\sigma_x + \frac{1}{\sqrt{3}}\sigma_y + \frac{1}{\sqrt{3}}\sigma_z)\} \quad (\text{D.9})$$

$$U_2 \otimes I = e^{-i\frac{\pi}{4}} \exp\{i\frac{\pi}{4}\sigma_z \otimes I\}, \quad (\text{D.10})$$

which gives the duration time for local operations $\omega\tau_1 = \frac{\pi}{2} + \frac{\pi}{3} + \frac{\pi}{4}$. The duration time for two-qubit interaction $e^{i\frac{\pi}{4}\sigma_z^1\sigma_z^2}$ is given as $\omega\tau_2 = \frac{\pi}{4}$ by using the same normalization. The total time to make a CNOT gate is $\tau = \tau_1 + \tau_2 = \frac{4\pi}{3\omega}$.

Appendix E

Filtering technique

The filtering technique is introduced by [34] and improved by [35, 33, 28] which is inserted in the formulation with the fluence constraint.

The fluence is the integral of the summation of the magnitude of external fields:

$$\int_0^T \sum_k \varepsilon_k^2(t) dt = E_0, \quad (\text{E.1})$$

which can be fixed by introducing a term

$$J_2 = -\gamma \left(\int_0^T \sum_k \varepsilon_k^2(t) dt - E_0 \right) \quad (\text{E.2})$$

in the functional, where γ is a Lagrange multiplier. The corresponding numerical procedure is changed as

$$(6.41) \rightarrow \varepsilon^{(i+\frac{1}{2})}(t) = \frac{1}{\gamma^{(i)}} \text{Im Tr } V^{(i)\dagger}(t) \sigma U^{(i)}(t) \quad (\text{E.3})$$

$$(6.43) \rightarrow \varepsilon^{(i+1)}(t) = \frac{\gamma^{(i)}}{\gamma^{(i+1)}} \varepsilon^{(i+\frac{1}{2})}(t), \quad (\text{E.4})$$

$$\text{where} \quad \gamma^{(i+1)} = \gamma^{(i)} \sqrt{\frac{\int_0^T \sum_k (\varepsilon_k^{(i+\frac{1}{2})}(t))^2 dt}{E_0}}. \quad (\text{E.5})$$

The filtering procedure is defined as an operator acting for the field $\varepsilon(t)$ which gives new field $\mathcal{F}[\varepsilon(t)]$. We can insert this filter at the step (E.5)

$$\varepsilon^{(i+1)}(t) = \mathcal{F}[\varepsilon^{(k+\frac{1}{2})}(t)]. \quad (\text{E.6})$$

The spectral constraint is imposed by choosing

$$\varepsilon^{(i+1)}(t) = \mathcal{F}_{\text{FT}}^{-1} \left[f(\omega) \mathcal{F}_{\text{FT}} \left[\varepsilon^{(i+\frac{1}{2})}(t) \right] \right] \quad (\text{E.7})$$

where $\mathcal{F}_{\text{FT}}$ is the Fourier transformation and $f(\omega)$ is a filtering function. For example, we can choose

$$f(\omega) = e^{-\xi(\omega-\omega_0)^2} + e^{-\xi(\omega+\omega_0)^2}, \quad (\text{E.8})$$

which allows only the components of the field around the frequency $\pm\omega_0$.

Appendix F

Lower bound for QFT

To quantify the minimum time (or minimum action) to generate n -qubit gate, we consider the system without constraint. The duration time is measured by using the normalization condition for the Hamiltonian: $\text{Tr } H^2 = 2^n \omega^2$. The quantum Fourier transform:

$$U_{\text{QFT}} = \frac{1}{\sqrt{2^n}} \sum_{j=0}^{2^n-1} \sum_{k=0}^{2^n-1} \exp \frac{2\pi i j k}{2^n} |j\rangle \langle k| \quad (\text{F.1})$$

can be generated by a static Hamiltonian since there are no constraints (see Section 4.1). The eigenvalues of QFT operator are in the set $(1, -1, -i, i)$ with the multiplicities in Table F.1.

N	1	-1	i	$-i$
$4m$	$m+1$	m	m	$m-1$
$4m+1$	$m+1$	m	m	m
$4m+2$	$m+1$	$m+1$	m	m
$4m+3$	$m+1$	$m+1$	$m+1$	m

Table F.1: The multiplicities of the eigenvalues for $N \times N$ Fourier transform [48]. For the one-qubit QFT, also known as the Hadamard gate, we see the eigenvalues are 1 and -1 since $N = 2$ and $m = 0$. For $n \geq 2$ qubit QFT, we have $N = 2^n$ and $m = 2^n/4$, thus the multiplicities of the eigenvalues can be seen in the first line on the table.

Using the table F.1, QFT matrix is diagonalized as

$$U_{\text{QFT}} = W \exp[i\Lambda] W^\dagger, \quad (\text{F.2})$$

$$\Lambda = \text{diag}(\underbrace{0, \dots}_{m+1}, \underbrace{\pm\pi, \dots}_m, \underbrace{\frac{\pi}{2}, \dots}_m, \underbrace{\frac{-\pi}{2}, \dots}_{m-1}), \quad (\text{F.3})$$

where $4m = N = 2^n$ for $n \geq 2$ and W is a unitary matrix. The Hamiltonian to generate U_{QFT} up to phase χ is written as

$$HT = W(-\Lambda + 2\pi \text{diag}(\nu_1, \dots, \nu_N) + \chi I) W^\dagger, \quad (\text{F.4})$$

where ν_i are arbitrary integers. To minimize the duration time T , we quantify $\text{Tr}(HT)^2$, namely

$$(\omega T)^2 = \frac{1}{4m} \min_{\chi, \nu_i, \pm} \text{Tr}(\Lambda - 2\pi \text{diag}(\nu_1, \dots, \nu_N) - \chi I)^2 \quad (\text{F.5})$$

$$= \frac{1}{4m} \min_{\chi} \left\{ \begin{array}{l} (m+1)\chi^2 + m(\pi - \chi)^2 \\ + m(\frac{\pi}{2} - \chi)^2 + (m-1)(\frac{-\pi}{2} - \chi)^2 \end{array} \right\} \quad (\text{F.6})$$

$$= \frac{20m^2 - 8m - 1}{(8m)^2} \pi^2, \quad (\text{F.7})$$

which is achieved when we choose the phase: $\chi = \frac{1+2m}{8m}\pi$. Thus, we have

$$(\omega T)^2 = \left(\frac{\pi}{2}\right)^2 \left(\frac{5}{4} - \frac{1}{2^{n-1}} - \frac{1}{2^{2n}}\right) \quad (\text{F.8})$$

for $n \geq 2$ (see Figure F.1).

In Section 6.8, we have seen that the duration time to generate n -qubit QFT gate by the Hamiltonian (6.68) is increased with the number of qubits, in spite of that the amplitude of the Hamiltonian is increased with n . On the other hand, the lower bound of the duration time for n -qubit QFT derived in this section is converging to a certain value for large n . This means that the restriction for the interactions in the model considered in Section 6.8 is too tight, e.g. there are no direct coupling between the j -th qubit and the $(j+2)$ -th qubit.

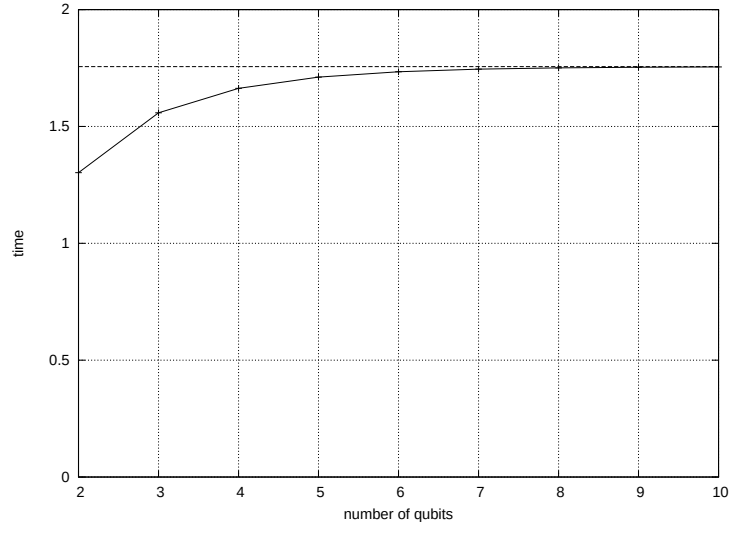


Figure F.1: The minimum time ωT to generate n -qubit QFT by the Hamiltonian normalized by $\text{Tr } H^2 = 2^n \omega^2$. The dotted line is $\frac{\sqrt{5}}{4}\pi \simeq 1.756$.

Bibliography

- [1] R. P. Feynman, *Foundations of Physics* **16**, 6 (1986).
- [2] D. Deutsch, *Proc. R. Soc. Lond. A*, **400**, 96 (1985).
- [3] D. Deutsch, *Proc. R. Soc. Lond. A*, **425**, 73 (1989).
- [4] P. W. Shor, in *Proceedings of the 35th Annual Symposium on the Foundation of Computer Science* (IEEE Computer Society Press, New York, 1994), p. 124.
- [5] L. K. Grover, in *Proceedings of the 28th Annual ACM Symposium on the Theory of Computing* (ACM Press, New York), p. 212 (1996); *Phys. Rev. Lett.*, **79**, 325 (1997).
- [6] J. R. Petta, A. C. Johnson, J. M. Taylor, E. A. Laird, A. Yacoby, M. D. Lukin, C. M. Marcus, M. P. Hanson and A. C. Gossard, *Science*, **309**, 2180 (2005).
- [7] Y. Makhlin, G. Schön, and A. Shnirman, *Rev. Mod. Phys.* **73**, 357 (2001).
- [8] A. O. Niskanen, Y. Nakamura and J.-S. Tsai, *Phys. Rev.* **B73**, 094506 (2006).
- [9] P. W. Shor, *Phys. Rev. A*, **52**, 2493 (1995).
- [10] A. Ekert and C. Macchiavello, *Phys. Rev. Lett.* **77**, 2585, (1996).
- [11] D. Gottesman, *Phys. Rev. A* **54**, 1862 (1996).
- [12] P. Zanardi and M. Rasetti, *Phys. Rev. Lett.*, **79**, 3306 (1997).
- [13] M. Reck, A. Zeilinger, H. J. Bernstein and P. Bertani, *Phys. Rev. Lett.* **73**, 58 (1994).

- [14] D. P. DiVincenzo, Phys. Rev. A **51**, 1015 (1995).
- [15] M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information*, (Cambridge University Press, Cambridge, U.K., 2000).
- [16] C. B. Boyer, *A History of Mathematics*, (Princeton University Press, Princeton, New Jersey, 1968).
- [17] A. P. Pirce, M. A. Dahleh and H. Rabitz, Phys. Rev. A **37**, 4950 (1988).
- [18] N. Khaneja and S.J. Glaser, Chem. Phys. **267**, 11 (2001); N. Khaneja, R. Brockett and S.J. Glaser, Phys. Rev. A **63**, 032308 (2001).
- [19] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley Phys. Rev. A **67**, 042313 (2003), *ibid* **69**, 042309 (2004).
- [20] J. Zhang, J. Vala, S. Sastry, and K. B. Whaley Phys. Rev. Lett. **91**, 027903 (2003); *ibid* **93**, 020502 (2004).
- [21] V. Ramakrishna, M. V. Salapaka, M. Dahleh, H. Rabitz and A. Peirce, Phys. Rev. A **51**, 960 (1995).
- [22] A. Carlini, A. Hosoya, T. Koike and Y. Okudaira, Phys. Rev. Lett. **96**, 060503 (2006).
- [23] A. Carlini, A. Hosoya, T. Koike and Y. Okudaira, Phys. Rev. A **75**, 042308 (2007).
- [24] A. Carlini, A. Hosoya, T. Koike and Y. Okudaira, J. Phys. A **41**, 045303 (2008).
- [25] J. Anandan and Y. Aharonov, Phys. Rev. Lett. **65**, 1697 (1990).
- [26] N. Margolus and L. B. Levitin, Physica D **120**, 188 (1998).
- [27] S. G. Schirmer, H. Fu, and A. I. Solomon, Phys. Rev. A **63**, 063410 (2001).
- [28] J. Werschnik and E. K. U. Gross, arXiv:0707.1883.
- [29] D. J. Tannor, V. A. Kazakov and V. Orlov, in *Time-Dependent Quantum Molecular Dynamics*, edited by J. Broeckhove and L. Lathouwers, NATO ASI, Ser. B (Plenum, New York, 1992), p. 347.

- [30] J. Somoloi, V. A. Kazakov and D. J. Tannor, Chem. Phys. **172**, 85 (1993).
- [31] J. P. Palao and R. Kosloff, Phys. Rev. Lett. **89**, 188301 (2002).
- [32] W. Zhu, J. Bonita, and H. Rabitz, J. Chem. Phys. **108**, 1953 (1998).
- [33] W. Zhu, and H. Rabitz, J. Chem. Phys. **109**, 385 (1998).
- [34] P. Gross, D. Neuhauser, and H. Rabitz, J. Chem. Phys., **96**, 2834 (1991).
- [35] T. Hornung, M. Motzkus and R. de Vivie-Riedle, J. Chem. Phys., **115**, 3105 (2001)
- [36] V. Giovannetti, S. Lloyd and L. Maccone, Phys. Rev. A **67**, 052109 (2003).
- [37] V. Giovannetti, S. Lloyd and L. Maccone, arXiv:quant-ph/0303085.
- [38] V. Giovannetti, S. Lloyd and L. Maccone, Europhys. Lett. **62**, 615, (2003).
- [39] A. Borrás, M. Casas, A. R. Plastino and A. Plastino, Phys. Rev. A **74**, 022326 (2006).
- [40] T. Hayashi, T. Fujisawa, H.D. Cheong, Y.H. Jeong and Y. Hirayama, Phys. Rev. Lett. **91**, 226804 (2003).
- [41] R. Hanson and G. Burkard, Phys. Rev. Lett. **98**, 050502 (2007).
- [42] H. P. Breuer and F. Petruccione, *The theory of open quantum systems* (Oxford University Press, Oxford, 2002).
- [43] S. E. Sklarz, D. J. Tannor and N. Khaneja, Phys. Rev. A **69**, 053408 (2004).
- [44] M. A. Nielsen, M. R. Dowling, M. Gu and A. C. Doherty, Science **311**, 1133 (2006).
- [45] M. A. Nielsen, M. R. Dowling, M. Gu and A. C. Doherty, Phys. Rev. A **73**, 062323.

- [46] M. R. Dowling and M. A. Nielsen, [arXiv:quant-ph/0701004](#).
- [47] A. Miyake and M. Wadati, *Phys. Rev. A*, **64**, 042317 (2001).
- [48] J. H. McClellan and T. W. Parks, *IEEE Transactions on Audio and Electroacoustics*, **20**, 66 (1972)

Publications

- Alberto Carlini, Akio Hosoya, Tatsuhiko Koike and Yosuke Okudaira, “Time-optimal quantum evolution”, *Physical Review Letters* **96**, 060503 (2006).
- Alberto Carlini, Akio Hosoya, Tatsuhiko Koike and Yosuke Okudaira, “Time-optimal unitary operations”, *Physical Review A* **75**, 042308 (2007).
- Alberto Carlini, Akio Hosoya, Tatsuhiko Koike and Yosuke Okudaira, “Time optimal quantum evolution of mixed states”, *Journal of Physics A: Mathematical and Theoretical* **41**, 045303 (2008).