Time Optimal Quantum Operartion for Mixed States

Alberto Carlini,^{1,*} Akio Hosoya,^{1,†} Tatsuhiko Koike,^{2,‡} and Yosuke Okudaira^{1,§}

¹Department of Physics, Tokyo Institute of Technology, Tokyo, Japan

²Department of Physics, Keio University, Yokohama, Japan

(Dated: January 26, 2007)

We formulate a variational principle for finding the time-optimal quantum evolution of mixed states subject to a master equation, when the Hamiltonian H and the Lindblad operators L_j are subject to certain constraints. We show that the problem can be reduced to solving first a fundamental equation (the "quantum brachistochrone") for H(t), which can be written down once the constraints are specified, and then solving the constraints and the master equation for the $L_j(t)$ s and the density operator $\rho(t)$. As an application of our formalism, we analytically solve a simple one qubit model where the optimal Lindblad operators correspond either to a measurement or to a decoherence process by the environment.

PACS numbers:

I. INTRODUCTION

Quantum control theory of pure states has been studied by many people (for an excellent review of the subject, see, e.g., [1]). For the mixed state case, the master equation in the Lindblad form has been used in [10]. A natural problem to investigate is the optimal quantum control of such systems. Around twenty years ago, Peirce, Dahleh and Rabitz [2] considered a variational method to manufacture a wave packet as close as possible to a target wave packet starting from a given initial wave packet. In our previous work we have established a general theory based on the variational principle to find a (time) optimal Hamiltonian which transforms a given initial state to a target state [26], and to find the (time) optimal unitary operation for arbitrary initial states [27] which is more relevant for quantum computation, where the input may be unknown. Recently, many works related to time optimal quantum computation have appeared in the literature [15–18, 20–25] (for a review see, e.g., [27]). The minimization of physical time to achieve a given unitary transformation provides a more physical description of the complexity of quantum algorithms.

Here we extend our previous works [26, 27] on the time optimal unitary evolution for pure quantum states and we formulate a variational principle for the time optimal quantum control of open systems where the dynamics is driven by a master equation in Lindblad [12, 13] form:

$$\frac{d\rho}{dt} := \mathcal{L}(\rho) = -i[H,\rho] + \sum_{j} (L_j \rho L_j^{\dagger} - \frac{1}{2} \{L_j^{\dagger} L_j,\rho\}), \quad (1)$$

for the density operator $\rho(t)$, where H(t) is the Hamiltonian, $L_j(t)$ $(j = 1, ..., N^2 - 1)$ are the Lindblad operators

and N is the dimension of the Hilbert space of the system. The Hamiltonian represents the unitary evolution part while the Lindblad operators express generalized measurements or decoherence processes due to the coupling of the system with an environment. Note that H(t) and $L_i(t)$ are considered here as dynamical variables evolving in time, besides the usual time dependent $\rho(t)$. The master equation is a Markovian, i.e. zero memory evolution equation that defines a quantum mechanical semigroup, and it can be physically realized if the interaction between the main physical system and with the environment is weak and the interaction time is small compared with the typical time scale of the physical system. The Hamiltonian and the Lindblad operators are constrained by some conditions due to physical laws or the experimental set-up. E.g., a normalization constraint for the Hamiltonian is necessary because one can afford only a finite amount of energy in experiments. The condition on the Lindblad operators is necessary because at least one should know the worst noise (i.e. decoherence rate) to perform any sensible experiment.

Note that the authors of [14] also considered the problem of control in dissipative quantum dynamics in order to achieve optimal purification of a quantum state, but they worked within the standard framework of a set of constant Lindblad operators. Furthermore, although there should be no conceptual difficulty in extending our work to the problem of optimal quantum control via quantum feedback by introducing a stochastic term in the master equation [5, 7, 8], we will not discuss this problem here.

The paper is organized as follows. In Section II we introduce the problem by defining an action principle for the time optimal unravelling of an open system under the condition that the evolution is driven by a master equation in Lindblad form and of the existence of a set of constraints for the available Hamiltonians and Lindblad operators, and we derive the fundamental equations of motion. In Section III we explicitly show how our theory via the example of a one-qubit system and we derive the time optimal Hamiltonian, which generates the uni-

^{*}Electronic address: carlini@th.phys.titech.ac.jp

[†]Electronic address: ahosoya@th.phys.titech.ac.jp

[‡]Electronic address: koike@phys.keio.ac.jp

SElectronic address: okudaira@th.phys.titech.ac.jp

tary evolution part of the density operator, and the time optimal Lindblad operators, which can represent either a measurement or a decoherence process by the environment. Finally, Section IV is devoted to the summary and discussion of our results.

II. A VARIATIONAL PRINCIPLE

Let us consider the problem of making the transition from a given initial state to a target state in the shortest time by controlling a certain physical system. We assume that the mixed state is governed by the master equation (1) with the traceless Hamiltonian H and the traceless Lindblad operators $\{L_i\}$. Mathematically this is a time optimality problem for the evolution of the density matrix $\rho(t)$ according to (1) and by controlling the Hamiltonian and the Lindblad operators. We assume that at least the 'magnitude' of the Hamiltonian and of the Lindblad operators is bounded. Physically this corresponds to the fact that one can afford only a finite energy in the experiment, and that a maximum level of noise is tolerated. Besides this normalization constraint, the available operations may be subject also to other constraints, which can represent either experimental requirements (e.g., the specifications of the apparatus in use) or theoretical conditions (e.g., allowing no operations involving three or more qubits). The mixed state is represented by an Ndimensional positive definite matrix, $\rho \in \mathcal{M}_N$, whose trace is preserved through the evolution by the master equation. We then define the following action for the dynamical variables $\rho(t)$, H(t) and $\{L_j(t)\}$.

$$S = \int dt \left\{ c(\rho, H, L_j) + \operatorname{Tr} \left[\sigma(\dot{\rho} - \mathcal{L}(\rho)) \right] \right.$$

+ $\frac{1}{2} \lambda_0 (\operatorname{Tr} H^2 - N\omega^2) + \sum_j \frac{1}{2} \lambda_j (\operatorname{Tr} L_j^{\dagger} L_j - N\gamma_j^2) \right\} (2)$

where the first term gives the time duration as the cost when we choose c = 1, the second term guarantees that the quantum evolution is governed by the master equation through the Lagrange multiplier σ , while the third and fourth terms constrain the amplitude of the Hamiltonian H and of the Lindblad operators $\{L_j\}$ through the Lagrange multipliers $\{\gamma_j\}$. The operator σ is traceless because the master equation does not contain the trace part. Therefore, taking variations of the action with respect to G and the traceless part of ρ , we obtain:

$$\dot{\rho} = \mathcal{L}(\rho) \tag{3}$$

$$\dot{\sigma} = i[\sigma, H] - P\left[\sum_{j} \left(L_{j}^{\dagger}\sigma L_{j} + \frac{1}{2}\{\sigma, L_{j}^{\dagger}L_{j}\}\right)\right], \quad (4)$$

where $P(X) = X - \frac{I}{N} \operatorname{Tr} X$ is a projection from $X \in \mathcal{M}_N$ to the traceless part of X. Furthermore, variations with respect to H and L_i^{\dagger} give

$$-i[\rho,\sigma] = \lambda_0 H \tag{5}$$

$$P\left(\sigma L_j \rho - \frac{1}{2} L_j \{\rho, \sigma\}\right) = \lambda_j L_j. \tag{6}$$

III. ONE QUBIT EXAMPLE

For a one-qubit system, the equations above can be decomposed into three dimensional vector equations by using the Pauli basis $\{\sigma_x, \sigma_y, \sigma_z\}$. Namely, we have $\rho = \frac{1}{2} + \mathbf{r} \cdot \boldsymbol{\sigma}, \, \sigma = \mathbf{s} \cdot \boldsymbol{\sigma}, \, H = \mathbf{h} \cdot \boldsymbol{\sigma}$ and $L_j = \mathbf{l}_j \cdot \boldsymbol{\sigma}$ where \mathbf{r}, \mathbf{s} and $\mathbf{h} \in \mathbb{R}^3$ and $\mathbf{l}_j \in \mathbb{C}^3$. According to this notation, the set of equations (1), (4), (5) and (6) can be rewritten as follows:

$$\dot{\boldsymbol{r}} = 2\boldsymbol{h} \times \boldsymbol{r} + \sum_{\boldsymbol{l}} (2\operatorname{Re}((\boldsymbol{l} \cdot \boldsymbol{r})\boldsymbol{l}^*) - 2|\boldsymbol{l}|^2 \boldsymbol{r} + i\boldsymbol{l} \times \boldsymbol{l}^*) \quad (7)$$

$$\dot{\boldsymbol{s}} = 2[\boldsymbol{h} \times \boldsymbol{s} - \sum_{\boldsymbol{l}} (\operatorname{Re}((\boldsymbol{l} \cdot \boldsymbol{s})\boldsymbol{l}^*) - |\boldsymbol{l}|^2 \boldsymbol{s})] \quad (8)$$

$$= 2[\mathbf{h} \times \mathbf{s} - \sum_{l} (\operatorname{Re}((\mathbf{l} \cdot \mathbf{s})\mathbf{l}^{*}) - |\mathbf{l}|^{2}\mathbf{s})]$$
(8)

$$\boldsymbol{r} \times \boldsymbol{s} = \lambda_0 \boldsymbol{h} \tag{9}$$

$$(\boldsymbol{s} \cdot \boldsymbol{l}_j)\boldsymbol{r} + (\boldsymbol{r} \cdot \boldsymbol{l}_j)\boldsymbol{s} + \boldsymbol{i}\boldsymbol{s} \times \boldsymbol{l}_j = \nu_j \boldsymbol{l}_j, \qquad (10)$$

where $\nu_j := \mathbf{r} \cdot \mathbf{s} + \lambda_j$. When \mathbf{r} and \mathbf{s} are not parallel, the components of the Hamiltonian \mathbf{h} are given by

$$\boldsymbol{h} = \pm \omega \frac{\boldsymbol{r} \times \boldsymbol{s}}{|\boldsymbol{r} \times \boldsymbol{s}|} \tag{11}$$

because of the constraint Tr $H^2 = 2\omega^2$. Using the master equation (7), (8) and the eigenvalue equation (10), one can see that

$$\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{r}\times\boldsymbol{s}) = 2\boldsymbol{h}\times(\boldsymbol{r}\times\boldsymbol{s}) \tag{12}$$

which, together with (9), guarantees the conservation of the vector $\mathbf{r} \times \mathbf{s}$.

Components of the Lindblad operators $\{l_j\}$ are determined as eigenvectors of the eigenvalue equation (10) with constraints $|l_j| = \gamma_j$. In some instant, we can parametrize r and s as

$$r = r(\cos\frac{\theta}{2}e_x + \sin\frac{\theta}{2}e_y)$$
 (13)

$$s = s(\cos\frac{\theta}{2}\boldsymbol{e}_{x} - \sin\frac{\theta}{2}\boldsymbol{e}_{y})$$
 (14)

where $r \cdot s = rs \cos \theta$ with the range $r \in [0, \frac{1}{2}]$ and $\theta \in [0, \pi]$, and rewrite (10) as

$$\begin{bmatrix} 2rs\cos^2\frac{\theta}{2} & 0 & -is\sin\frac{\theta}{2} \\ 0 & -2rs\sin^2\frac{\theta}{2} & -is\cos\frac{\theta}{2} \\ is\sin\frac{\theta}{2} & is\cos\frac{\theta}{2} & 0 \end{bmatrix} l_j = \lambda_j l_j. \quad (15)$$

If the initial conditions satisfy $r(0) \times s(0) = 0$, then we also have $r(t) \times s(t) = 0$ because of (12), and the components of the Lindblad operators are given by (15) as the following constants:

$$\boldsymbol{l}_{\pm} = \frac{\gamma_{\pm}}{\sqrt{2}} (\boldsymbol{e}_{\boldsymbol{x}} \pm i \boldsymbol{e}_{\boldsymbol{y}}) \tag{16}$$

$$\boldsymbol{l}_0 = \gamma_0 \boldsymbol{e}_{\boldsymbol{z}}, \qquad (17)$$

where e_z is the unit vector parallel to r. Since the Hamiltonian cannot be zero, except for the case of $\omega = 0$, from (11) we see that $\lambda_0 = 0$ and h is arbitrary. To get rid of the effect of the Hamiltonian, we move to the interaction picture by the transformation $\rho' = U_0 \rho U_0^{\dagger}$ with $U_0(t) = \mathcal{T} \exp(-i \int H(t) dt)$. In the new frame, the master equation reads

$$\dot{\boldsymbol{r}} = \sum_{\boldsymbol{l}} [2\operatorname{Re}(\boldsymbol{l} \cdot \boldsymbol{r})\boldsymbol{l}^* - 2|\boldsymbol{l}|^2 \boldsymbol{r} + i\boldsymbol{l} \times \boldsymbol{l}^*], \qquad (18)$$

and for the initial conditions as above we have

$$\dot{\boldsymbol{r}} = -2(\gamma_+^2 + \gamma_-^2)\boldsymbol{r} + (\gamma_+^2 - \gamma_-^2)\boldsymbol{e_z}$$
 (19)

which guarantees $\dot{e}_{z} = 0$. Therefore we obtain the following solution for the components of the density operator

$$\boldsymbol{r}(t) = \left\{ \frac{(\gamma_+^2 - \gamma_-^2)}{2(\gamma_+^2 + \gamma_-^2)} + C e^{-2(\gamma_+^2 + \gamma_-^2)t} \right\} \boldsymbol{e}_{\boldsymbol{z}}.$$
 (20)

Choosing magnitudes of the Lindblad operators as $\gamma_+ = \gamma_-$, the state will just lose the coherence, but the coherence can be recovered when magnitudes of the Lindblad operators are different (see fig.1).



FIG. 1: Analytical, time optimal evolution of $\rho(t)$ in the Bloch sphere for the case of $\mathbf{r} \times \mathbf{s} = \mathbf{0}$ with a constant Hamiltonian $H = \mathbf{h} \cdot \boldsymbol{\sigma}, \ \gamma_+ \neq 0, \ \gamma_- = \gamma_0 = 0 \text{ and } \rho(0) = (1 + \sigma_z)/2.$

- M. Shapiro and P. Brumer, Principles of of the Quantum Control of Molecular Processes (Wiley & Sons, New York, 2003).
- [2] A.P. Peirce, M.A. Dahleh and H. Rabitz, *Phys. Rev.* A37, 4950 (1988).
 [3] D.J. Tannor and S.A. Rice, *J. Chem. Phys.* 83, 5013
- [3] D.J. Tannor and S.A. Rice, J. Chem. Phys. 83, 5013 (1985).
- [4] J.P. Palao and R. Kosloff, Phys. Rev. A68, 062308 (2003).
- [5] V.P. Belavkin, Information, Complexity and Control in Quantum Physics (eds. A. Blaquiere, S. Dinar and G. Lochak, Springer Verlag, New York, 1987); V.P. Belavkin, Comm Math. Phys. 146, 611 (1992).
- [6] H.M. Wiseman and G.J. Milburn, Phys. Rev. Lett. 70, 548 (1993).
- [7] S. Mancini and H.M. Wiseman, quant-ph/0610006.
- [8] H.M. Wiseman and A.C. Doherty, Phys. Rev. Lett. 94, 070405 (2005).
- [9] H.M. Wiseman and K. Jacobs, Phys. Rev. A60, 2700 (1999).
- [10] S. Lloyd and L. Viola, quant-ph/0008101; S. Lloyd and L. Viola, Phys. Rev. A65, 010101(R) (2001).

IV. SUMMARY AND DISCUSSION

We have developed a framework for finding the time optimal quantum operation to transform a given pure or mixed state to another, when the physical system obeys a Markovian master equation in Lindblad form. The equations for the Hamiltonian H and the Lindblad operator L_a can be written down once the constraints for H and L_a are specified according to the problem. One then obtains the time optimal operation $(H(t), L_a(t))$ and the optimal time duration T by solving the equations and imposing the initial and final conditions $\rho(0) = \rho_i$ and $\rho(T) = \rho_f$.

We have presented a single qubit model to demonstrate our variational formalism of the quantum brachistochrone for the mixed state case. The optimal Hamiltonian is obtained by solving the quantum brachistochrone equation and then a set of ordinary differential equations give the time evolution of the density operator together with the Lindblad operators which represent the optimal non-unitary operations corresponding to a measurement or to decoherence. In a particular case, an analytical solution was given. The full version of this work can be seen in [28]

ACKNOWLEDGEMENTS

This research was partially supported by the MEXT of Japan, under grant No. 09640341 (A.H. and T.K.), by the JSPS with grant L05710 (A.C.), by the COE21 project on 'Nanometer-scale Quantum Physics' at Tokyo Institute of Technology and by Macquarie University (A.C.).

- [11] R. Wu, A. Pechen, C. Brif and H. Rabitz, quantph/0611215.
- [12] G. Lindblad, Comm. Math. Phys. 48, 199 (1976).
- [13] V. Gorini, A. Kossakowski and E.C.G. Sudarshan, J. Math. Phys. 17, 821 (1976).
- [14] S.E. Sklarz, D.J. Tannor and N. Khaneja, Phys. Rev. A69, 053408 (2004).
- [15] N. Khaneja and S.J. Glaser, *Chem. Phys.* 267, 11 (2001);
 N. Khaneja, R. Brockett and S.J. Glaser, *Phys. Rev.* A63, 032308 (2001).
- [16] G. Vidal, K. Hammerer and J.I. Cirac, *Phys. Rev. Lett.* 88, 237902 (2002); id., *Phys. Rev.* A66, 062321 (2002); J. Zhang, J. Vala, S. Sastry and K.B. Whaley, *Phys. Rev.* A67, 042313 (2003).
- [17] T. Schulte-Herbrüggen, A. Spörl, N. Khaneja and S.J. Glaser, Phys. Rev. A72, 042331 (2005).
- [18] U. Boscain and P. Mason, J. Math. Phys. 47, 062101 (2006).
- [19] M.A. Nielsen and I.L. Chuang, Quantum Computation and Quantum Information (Cambridge University Press, Cambridge, 2000).
- [20] S. Tanimura, M. Nakahara and D. Hayashi, J. Math.

Phys. 46, 022101 (2005).

- [21] M.A. Nielsen, M. Dowling, M. Gu and A. Doherty, Science 311, 1133 (2006).
- [22] M.A. Nielsen, M.R. Dowling, M. Gu and A.C. Doherty, *Phys. Rev.* A73, 062323 (2006).
- [23] M.A. Nielsen, Quant. Inf. Comput. 6, 213 (2006).
- [24] M. Dowling and M. A. Nielsen, quant-ph/0701004.
- [25] N. Khaneja, B. Heitmann, A. Spörl, H. Yuan, T. Schulte-Herbrüggen and S.J. Glaser, quant-ph/0605071.
- [26] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, Phys. Rev. Lett. 96, 060503 (2006).
- [27] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, quantph/0608039. to appear Phys.Rev.A 75(2007)
- [28] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, "Quantum Brachistochrone for Mixed States" quantph/0703047.