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Alberto Carlini[1], Akio Hosoya[2], Tatsuhiko Koike[3] and Yosuke Okudaira[2]

[1] Centre for Quantum Computer Technology, Department of Physics, Macquarie University, Sydney, Australia
[2] Department of Physics, Tokyo Institute of Technology, Tokyo, Japan
[3] Department of Physics, Keio University, Yokohama, Japan

E-mail: carlini@ics.mq.edu.au, ahosoya@th.phys.titech.ac.jp, koike@phys.keio.ac.jp and okudaira@th.phys.titech.ac.jp

Abstract

We present a general formalism based on the variational principle for finding the time-optimal quantum evolution of mixed states governed by a master equation, when the Hamiltonian and the Lindblad operators are subject to certain constraints. The problem may be reduced to solving first a fundamental equation, which can be written down once the constraints are specified, for the Hamiltonian and then solving the constraints and the master equation for the Lindblad and the density operators. As an application of our formalism, we study a simple one-qubit model, where the optimal Lindblad operators can be simulated by a tunable coupling with an ancillary qubit.

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1. Introduction

Recently, many works related to time optimal quantum computation have appeared in the literature [1–11]. The minimization of physical time to achieve a given unitary transformation should provide a more physical description of the complexity of quantum algorithms. In a series of previous works [12, 13], we established a general theory based on the variational principle to find the time optimal evolution between the given initial and final pure states [12] (paper I), and to find the time optimal way of generating a target unitary operation for arbitrary initial states [13] (paper II). In paper I, we studied closed pure quantum systems driven by the Schrödinger equation and where the Hamiltonian is controllable within a certain available set. Paper II is an extension of paper I and is more relevant to subroutines in quantum computation, where the input may be unknown. The main result of our works is that, once the constraints for the Hamiltonian are given, one can systematically derive a fundamental equation (which we call the *quantum brachistochrone*) that can always be solved, at least numerically, for the

time optimal Hamiltonian (without any further restricting assumptions, e.g. the adiabaticity of the quantum evolution).

Here we extend our previous works and formulate a variational principle for the time optimal control of the evolution of quantum mixed states in open systems, where the dynamics is driven by a master equation in the Lindblad form [14, 15]. The Lindblad operators in the master equation describe non-unitary evolution, which can be called decoherence if it is not controllable and a measurement if it is controllable. It is interesting to note that sometimes measurements can accelerate the state evolution to the desired final state[4]. In this work, we discuss the time optimal evolution of a mixed state by controlling the Hamiltonian and the Lindblad operators.

Historically, quantum control theory of pure states has been studied by many people (for a review of the subject, see, e.g., [16]). Around 20 years ago, Peirce, Dahleh and Rabitz [17] considered a variational method to manufacture a wave packet as close as possible to a given target. Other authors (see, e.g., [18] and other references in [16]) further investigated the variational methods by optimizing the fidelity between the final state of the steered system and a given target state. The application to the optimal realization of unitary gates in closed systems was also studied (see, e.g., [19]). For the case of quantum mixed states, the master equation in the Lindblad form has been used in many works [20–22]. However, while the main concern of these papers was the optimization of the fidelity or the purity of the quantum operations, here we focus the attention on the time optimality. Furthermore, we concentrate on the problem of state evolution, i.e., the present work is a direct extension of paper I to the case of mixed states. Although the Lindblad operators are usually treated in the context of decoherence and assumed to be uncontrollable, there are some works which discuss controllable Lindblad operators (e.g. [23]).

The paper is organized as follows. In section 2, we introduce the Markovian approximation and the master equation for an open quantum system. In section 3, we set up the general variational formalism for finding the time optimal evolution between the given initial and final states of such an open system. The action consists of a time-cost function to be minimized and of Lagrange multiplier terms which ensure the state evolution under the master equation and certain constraints for the available Hamiltonian and Lindblad operators. We then derive the fundamental equations of motion. In section 4 we explicitly demonstrate our methods via the example of a one-qubit system by deriving the time optimal Hamiltonian, Lindblad and density operators, which may represent either a measurement or a decoherence process. In section 5, we simulate the optimal operations derived in section 4 by the partial trace of a two-qubit self-interacting system with a controllable Hamiltonian and ancillary qubit. This corresponds to a repetition of short-time measurements. Finally, section 6 is devoted to the summary and discussion of our results, while in the appendix we discuss the gauge degrees of freedom of the master equation.

2. Master equation

In this paper, we address the problem of time optimal quantum control of open systems where the dynamics is described by a master equation in the Lindblad form [14, 15]

$$\dot{\rho} = \mathcal{L}(\rho) := -\mathrm{i}[H, \rho] + \sum_a \left(L_a \rho L_a^\dagger - \frac{1}{2} \{ L_a^\dagger L_a, \rho \} \right) \tag{1}$$

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[4] This can be seen by the simple example of a photon counter. Suppose that the system can be in two states specified by the number of photons, zero and one. By absorbing a photon, the photon counter changes the state $|1\rangle$ to $|0\rangle$ and leaves $|0\rangle$ unchanged. This can be used to accelerate the transition to the state $|0\rangle$.

for the density operator $\rho(t)$, where $H(t)$ is the Hamiltonian, $L_a(t)$ ($a = 1, \ldots, N^2 - 1$) are the Lindblad operators, N is the dimension of the Hilbert space of the system and we use the notation $\dot{A} := dA/dt$ for time derivatives, $[A, B] := AB - BA$ for the commutator and $\{A, B\} := AB + BA$ for the anticommutator. 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. The master equation is Markovian, i.e. the environment has no memory of the main physical system. It can be physically realized, if the interaction between the main system and the environment is weak and its typical time scale is small compared with that of the physical system [24, 25]. A simple example discussed in section 5 illustrates how the repetition of a short time unitary evolution and the partial trace (e.g., measurement) over the environment states (35) reproduces the master equation (1).

From the gauge freedom of the master equation (1) (see the appendix), we can always choose $H = \widetilde{H}, L_a = \widetilde{L}_a$, where a tilde denotes the traceless part of an operator, $\widetilde{A} := A - (\text{Tr } A/N)\mathbb{1}$. Furthermore, by using the degrees of freedom of (A.2), we can also choose the L_a to be mutually orthogonal. This is the gauge choice which we make throughout this paper.

3. General formalism

Let us consider the problem of controlling a certain physical system governed by the master equation (1) and of steering its transition between given initial and final quantum states in the shortest time. Mathematically, this is a time optimality problem for the evolution of the density operator $\rho(t)$ according to (1) by controlling the Hamiltonian $H(t)$ and the Lindblad operators $L_a(t)$. We assume that at least the 'magnitudes' of the Hamiltonian and of the Lindblad operators are bounded. Physically, this corresponds to the fact that one can afford only a finite energy in the experiment, and that a finite level of decoherence 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).

We then consider the following action for the dynamical variables $\rho(t)$, $H(t)$ and $L_a(t)$:

$$S = \int_0^1 d\tau \, (\alpha + \text{Tr}[\sigma(\rho' - \alpha \mathcal{L}(\rho))] + L_C), \tag{2}$$

where

$$L_C := \sum_m \bar{\lambda}_m f_m(H) + \sum_{a,b} \bar{\mu}_{ab} \big[\text{Tr}(L_a^\dagger L_b) - N\gamma_a^2 \delta_{ab} \big]. \tag{3}$$

Let us explain the notation and the meaning of the various terms in (2) and (3). The parameter τ can be arbitrarily chosen as long as it satisfies the conditions $\rho(0) = \rho_i$ and $\rho(1) = \rho_f$, so that the action S is invariant under reparameterization of τ. The quantity α is the time cost. The traceless Hermitian operator $\sigma(t)$, the real functions $\bar{\lambda}_m(t)$ ($m = 0, \ldots, M - 1$) and the complex functions $\bar{\mu}_{ab}(t) = \bar{\mu}_{ba}^*(t)$ ($a, b = 1, \ldots, N^2 - 1$) are Lagrange multipliers, the real functions f_m are the constraints for the Hamiltonian, and $\gamma_a > 0$ are the decoherence rates or the measurement strengths. Furthermore, we denote $A' := dA/d\tau$. As mentioned in the previous section, we assume (even before taking variations of the action) that $\text{Tr } \rho(t) = 1$ and H and L_a are traceless[5].

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[5] Our results are unchanged if one explicitly introduces Lagrange multiplier terms in action (2) in order to ensure the trace conditions for the operators H, L_a, σ and ρ.

The first term in action (2) can be interpreted as either one of the following: (1) a positive independent dynamical variable, the lapse function, which measures the physical time lapsed in each infinitesimal interval $d\tau$ of the parameter time τ; or (2) any positive functional of the other dynamical variables ensuring that the action is reparameterization invariant and that $\int \alpha \, d\tau$ becomes the physical time t under the equations of motion. In the second case, α can be chosen for example to be $\sqrt{\frac{g_\rho(\rho',\rho')}{g_\rho(\mathcal{L}(\rho),\mathcal{L}(\rho))}}$, where g_ρ is any reasonable metric on the space of density operators, e.g., the Bures metric or more generally a Morozova–Chentsov–Petz monotone metric [27, 28]. This choice is motivated by the Anandan–Aharonov relation in the case of pure states and therefore yields a natural extension of paper I to the mixed states. However, here we choose the first option and take α as an independent dynamical variable, which makes the derivation of the equations of motion simpler.

The second term in action (2) guarantees that $\rho(t)$ satisfies the master equation (1). In fact, from the variation by σ, we obtain

$$\rho' - \alpha\mathcal{L}(\rho) = 0. \tag{4}$$

By defining $t := \int \alpha(\tau) \, d\tau$ and interpreting t as the physical time, the above equation is equivalent to the master equation (1), and the minimization problem of S becomes the optimization problem for the physical time.

The third term L_C in action (2) generates two types of constraints. The first set is obtained from the variation of S by $\bar{\lambda}_m$ and consists of the M constraints for the Hamiltonian,

$$f_m(H) = 0. \tag{5}$$

The second set, obtained from the variation of S by $\bar{\mu}_{ab}$, ensures the normalization and the mutual orthogonality of the L_a operators,

$$\mathrm{Tr}\big(L_a^\dagger L_b\big) = N\gamma_a^2 \delta_{ab}. \tag{6}$$

Although one can consider more general constraints for L_a, which is particularly important if controllable and uncontrollable Lindblad operators coexist, we restrict ourselves to the case (6) for the simplicity of the presentation. The extension to more general cases is straightforward.

Let us then derive the other equations of motion. From the variation of S by ρ, with the help of (1), one gets the adjoint master equation[6]

$$\dot{\sigma} = -\widetilde{\mathcal{L}^\dagger(\sigma)}, \tag{7}$$

where the superoperator $\mathcal{L}^\dagger$ is defined by $\mathrm{Tr}[A^\dagger \mathcal{L}(B)] = \mathrm{Tr}[\mathcal{L}^\dagger(A)B]$ and its explicit form is $\mathcal{L}^\dagger(A) = i[H, A] + \sum_a \big(L_a^\dagger A L_a - \frac{1}{2}\{L_a^\dagger L_a, A\}\big)$. The variation of S by H with the aid of (1) implies

$$F = -i[\rho, \sigma], \tag{8}$$

where we have defined a traceless operator

$$F(H) := \sum_m \lambda_m \frac{\partial f_m(H)}{\partial H}, \tag{9}$$

with $\lambda_m := \bar{\lambda}_m/\alpha$. From the variation of S by $L_a^\dagger$, together with (1), we obtain an algebraic equation (see footnote 6)

$$\text{traceless part of } \left[\sigma L_a \rho - \frac{1}{2}L_a\{\rho, \sigma\}\right] = \sum_b \mu_{ab} L_b, \tag{10}$$

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[6] Here, we have used the fact that the differential $\partial \bar{L}/\partial A$ of a scalar functional $\bar{L}$ by an operator A with fixed trace is traceless.

where $\mu_{ab} := \bar{\mu}_{ab}/\alpha$. One can show that μ_{ab} is actually diagonal, i.e. that $\mu_{ab} = \mu_a\delta_{ab}$ with real μ_a,[7] and therefore one gets

$$\text{traceless part of } \left[\sigma L_a\rho - \tfrac{1}{2}L_a\{\rho,\sigma\}\right] = \mu_a L_a, \tag{11}$$

which is an eigenvalue equation with eigenvalues μ_a for the eigenvectors L_a.

Combining (1), (7), (8) and (11) we can eliminate the Lagrange multipliers σ and μ_a[8] to obtain what we call the *quantum brachistochrone equation*

$$i\dot{F} = [H, F]. \tag{12}$$

Finally, the condition derived from the variation of S by α, i.e. $\text{Tr}\,\sigma\mathcal{L}(\rho) = 1$, merely determines the common scale for the (unphysical) Lagrange multipliers σ, λ_m and μ_{ab}.[9]

As a result, the time optimality problem reduces to the following set of equations for the variables $\rho(t)$, $H(t)$, $L_a(t)$, $\sigma(t)$, $\lambda_m(t)$ and $\mu_a(t)$: the master equation (1), the constraints (5) and (6), the adjoint master equation (7), the eigenvalue equation (11) and a choice between the quantum brachistochrone equation (12) or an algebraic equation (8) (with the definition (9)). The variable α has been absorbed completely.

We emphasize that the quantum brachistochrone equation (12) is the same and universal for pure states (paper I) and for unitary operations (paper II). In particular, (12) involves only the Hamiltonian operator H but not the Lindblad operators L_a.[10] Thus one can find $H(t)$ independently from $\rho(t)$ and $L_a(t)$. This is done by solving a closed set of equations for $H(t)$ and $\lambda_m(t)$, which consists of the quantum brachistochrone (12) and the algebraic equations (5) and (9). As for the initial values, $F(0)$ must be specified by ρ_i and some Hermitian operator $\sigma(0)$ through (8), and then $H(0)$ and $\lambda_m(0)$ are determined from (5) and (9).[11] Finally, to obtain the time evolution of $\rho(t)$ and $L_a(t)$, one must solve the remaining equations (1), (7) and (11), in a way similar to what is described below.

An alternative procedure, which may be practical for the numerical integration, is the following. Suppose the initial and final states ρ_i and ρ_f are given. One first specifies a trial initial value $\sigma(0)$. At each instant, if $\rho(t)$ and $\sigma(t)$ are known, one can algebraically find $F(t)$ from (8), $L_a(t)$ and $\mu_{ab}(t)$ from (6) and (11), and then $H(t)$ and $\lambda_m(t)$ from (5) and (9) (see footnote 11). Thus, starting from $\sigma(0)$ and $\rho(0) = \rho_i$, one can integrate the master equation (1) and the adjoint master equation (7). Finally, the whole procedure is repeated until one finds a good $\sigma(0)$ which generates the trajectory such that $\rho(T) = \rho_f$ for some $T > 0$. Besides this shooting method, there may be other numerical strategies [29].

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[7] With the help of the orthogonality condition (6) we can see from (10) that $N\mu_{ab}^2(\gamma_a^2 - \gamma_b^2) = \text{Tr}[(\sigma L_b\rho - \tfrac{1}{2}L_b\{\rho,\sigma\})L_a^\dagger - L_b(\sigma L_a^\dagger\rho - \tfrac{1}{2}\{\rho,\sigma\}L_a^\dagger)]$. The right-hand side of the latter formula is identically zero so that one can conclude that $\mu_{ab} = 0$ if $\gamma_a \neq \gamma_b$. For equal γ_a, one can still rotate (using (A.2)) the L_a and diagonalize μ_{ab}. In all cases, we obtain $\mu_{ab} = \mu_a\delta_{ab}$.

[8] Taking the derivative of (8) and using (1) and (7) we obtain $\dot{F} = -i[H, F] + i\sum_a([L_a\rho L_a^\dagger - \tfrac{1}{2}\{L_a^\dagger L_a, \rho\}]\sigma] + [L_a^\dagger\sigma L_a - \tfrac{1}{2}\{L_a^\dagger L_a, \sigma\}\rho])$. Then, inserting (11) and its adjoint, we obtain (12).

[9] By substituting (8) and the trace of '(11) times $L_a^\dagger$' into $\text{Tr}\,\sigma\mathcal{L}(\rho) = 1$, one finds $\text{Tr}\,HF = 1 - N\sum\mu_a\gamma_a^2$. This equation is, however, not independent of the other equations of motion, except for the initial values, so that we do not need to solve it. This can be seen by $(\text{Tr}\,HF)^{\cdot} = \text{Tr}\,\dot{H}F + \text{Tr}\,H\dot{F} = \sum_m\lambda_m\dot{f}_m - i\text{Tr}\,H[H, F] = 0$, where we have used definition (9) for F, the quantum brachistochrone equation (12) and the constraints (5). Then $\text{Tr}\,HF = 1 - N\sum\mu_a\gamma_a^2$ always holds if it does initially too. The condition can always be satisfied by a simultaneous rescaling of $\sigma(t)$, $\lambda_m(t)$ and $\mu_{ab}(t)$ under which all the other equations of motion are invariant.

[10] This is so because we assumed that the constraints for H and those for L_a are independent, as can be seen in (3) which is natural physically. In a more general case, where $L_C = \sum_m\bar{\lambda}_m f_m(H, L_a, L_a^\dagger)$, the RHS of (10) becomes $F_a^\dagger$ and (12) reads $i\dot{F} = [H, F] + \sum_a([L_a, F_a] + [L_a^\dagger, F_a^\dagger])$ where $F_a := \partial L_C/\partial L_a$, and hence the equations couple more severely. Note, however, that in many cases one still has $[L_a, F_a] = 0$ so that the quantum brachistochrone equation reduces to (12).

[11] The Hamiltonian $H(t)$ and the Lagrange multipliers $\lambda_m(t)$ have $N^2 - 1$ and M degrees of freedom, respectively. Thus they can be determined algebraically at each time t from the M equations (5) and the $N^2 - 1$ equations (9).

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

$$f_0(H) := \tfrac{1}{2}(\text{Tr}\, H^2 - 2\omega^2) = 0, \tag{13}$$

where ω is a given constant. In this case, $F = \lambda_0 H$ and the quantum brachistochrone equation (12) becomes trivial, giving $H = \text{const}$ and $\lambda_0 = \text{const}$ (see section 3 in paper II). Our problem then reduces to that of solving the master equation (1) and the adjoint master equation (7) together with the algebraic equations (8) and (11) 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 parameterize the states as

$$\rho(t) := \tfrac{1}{2}[\mathbb{1} + \boldsymbol{r}(t) \cdot \boldsymbol{\sigma}], \tag{14}$$

$$\sigma(t) := \boldsymbol{s}(t) \cdot \boldsymbol{\sigma}, \tag{15}$$

and the Hamiltonian and the Lindblad operators as

$$H := \boldsymbol{h} \cdot \boldsymbol{\sigma}, \tag{16}$$

$$L_a(t) := \boldsymbol{l}_a(t) \cdot \boldsymbol{\sigma}, \tag{17}$$

where $\boldsymbol{r}, \boldsymbol{s}$ and $\boldsymbol{h} \in \mathbb{R}^3$ and $\boldsymbol{l}_a \in \mathbb{C}^3$, the master equation (1) and the adjoint master equation (7) can be rewritten as

$$\dot{\boldsymbol{r}} = 2[\boldsymbol{h} \times \boldsymbol{r} + \sum_{l \in \{l_a\}} (\text{Re}((\boldsymbol{l} \cdot \boldsymbol{r})\boldsymbol{l}^*) - |\boldsymbol{l}|^2 \boldsymbol{r} + i\boldsymbol{l} \times \boldsymbol{l}^*)], \tag{18}$$

$$\dot{\boldsymbol{s}} = 2[\boldsymbol{h} \times \boldsymbol{s} - \sum_{l \in \{l_a\}} (\text{Re}((\boldsymbol{l} \cdot \boldsymbol{s})\boldsymbol{l}^*) - |\boldsymbol{l}|^2 \boldsymbol{s})]. \tag{19}$$

Moreover, the algebraic equations (8) and (11) read

$$\boldsymbol{r} \times \boldsymbol{s} = \lambda_0 \boldsymbol{h} = \text{const.} \tag{20}$$

and

$$K(\boldsymbol{r}, \boldsymbol{s})\boldsymbol{l}_a = \nu_a \boldsymbol{l}_a, \tag{21}$$

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

$$K_{jk}(\boldsymbol{r}, \boldsymbol{s}) := r_j s_k + r_k s_j - 2i \sum_{l=1,2,3} \epsilon_{jkl} s_l \tag{22}$$

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

Because of the constraints (13) and (20), the components of the Hamiltonian $\boldsymbol{h}$ are given by

$$\boldsymbol{h} = \begin{cases} \pm\omega \dfrac{\boldsymbol{r} \times \boldsymbol{s}}{|\boldsymbol{r} \times \boldsymbol{s}|} & \text{if} \quad \boldsymbol{r} \times \boldsymbol{s} \neq \boldsymbol{0}, \\ \omega\boldsymbol{n} & \text{if} \quad \boldsymbol{r} \times \boldsymbol{s} = \boldsymbol{0}, \end{cases} \tag{23}$$

where $\boldsymbol{n}$ is an arbitrary unit vector. The components of the Lindblad operators $\boldsymbol{l}_a$ are determined as eigenvectors of the eigenvalue equation (21) with the constraints (6), i.e. $|\boldsymbol{l}_a| = \gamma_a$.

At a given instant, we parameterize $r(t)$ and $s(t)$ as

$$r(t) := r \left(\cos \frac{\theta}{2} e_3 + \sin \frac{\theta}{2} e_1 \right), \tag{24}$$

$$s(t) := s \left(\cos \frac{\theta}{2} e_3 - \sin \frac{\theta}{2} e_1 \right), \tag{25}$$

where $\{e_1(t), e_2(t), e_3(t)\}$ are orthonormal vectors, so that $r \cdot s = rs \cos\theta$, with $r \in [0, 1]$ and $\theta \in [0, \pi]$. We can then rewrite the matrix K in (22) as

$$(K_{jk}) = 2s \begin{bmatrix} -r \sin^2 \frac{\theta}{2} & -i \cos \frac{\theta}{2} & 0 \\ i \cos \frac{\theta}{2} & 0 & i \sin \frac{\theta}{2} \\ 0 & -i \sin \frac{\theta}{2} & r \cos^2 \frac{\theta}{2} \end{bmatrix}. \tag{26}$$

If the conserved vector satisfies $r \times s = \mathbf{0}$, we can see that $\theta = 0$ (i.e. $r = re_3$), and the components of the Lindblad operators are given by (21) and (26) as the following vectors:

$$l_1(t) = \frac{\gamma_1}{\sqrt{2}}(e_1 + ie_2), \tag{27}$$

$$l_2(t) = \frac{\gamma_2}{\sqrt{2}}(e_1 - ie_2), \tag{28}$$

$$l_3(t) = \gamma_3 e_3. \tag{29}$$

To simplify the analysis, we can move to the interaction picture by the transformation $\bar\rho = U_0 \rho U_0^\dagger := \frac{1}{2}(\mathbb{1} + \bar{r} \cdot \sigma)$ with $U_0(t) = \mathcal{T} \exp(-i \int H(t) \, dt)$ ($\mathcal{T}$ is the time-ordered product), so that the master equation (18) becomes

$$\dot{\bar{r}} = -2 \left[(\gamma_1^2 + \gamma_2^2) \bar{r} - (\gamma_1^2 - \gamma_2^2) e_3 \right], \tag{30}$$

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

$$\bar{r}(t) = \left[\frac{\gamma_1^2 - \gamma_2^2}{\gamma_1^2 + \gamma_2^2} + \left(\bar{r}(0) - \frac{\gamma_1^2 - \gamma_2^2}{\gamma_1^2 + \gamma_2^2} \right) e^{-2(\gamma_1^2 + \gamma_2^2)t} \right] e_3. \tag{31}$$
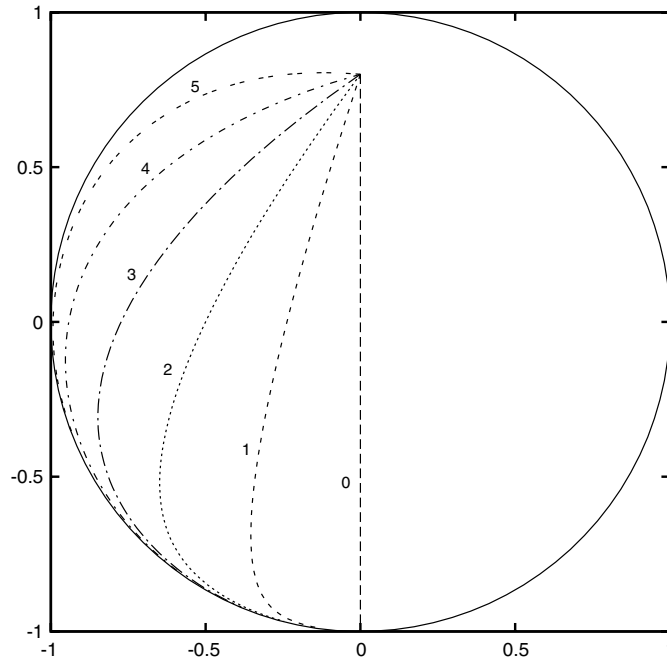
If the magnitudes of the Lindblad operators are equal, i.e. $\gamma_1 = \gamma_2$, the state will irretrievably lose the coherence, but the coherence can be recovered when the magnitudes of the Lindblad operators are different. Note that in this particular case the L_3 operator, which corresponds to a projective measurement along e_3, is not effective for the state evolution while the amplitude damping channels L_1 and L_2 play a significant role in (31). The case $h = \mathbf{0}$ is depicted in figure 1. In the case when $r \times s \neq 0$, the coupled equations (18), (19) and (21) can be solved numerically. We depict a family of optimal trajectories from a mixed state to a pure state in the Bloch sphere in figure 2.

As a final remark for this section we would like to point out that in order to make the time duration of the transition physically well-defined, one can introduce a small but finite error region around the target state. That is, one can be more interested in reaching the target state with a fixed fidelity close to one. Then, for example, while mathematically it takes an infinite time for the system to reach the target state, the system actually approaches the target state and enters into its small surrounding region in a finite time. In particular, in some cases the time optimal mixed state evolution can be faster than the time optimal pure state evolution (thick solid curve in figure 1) discussed in paper I.
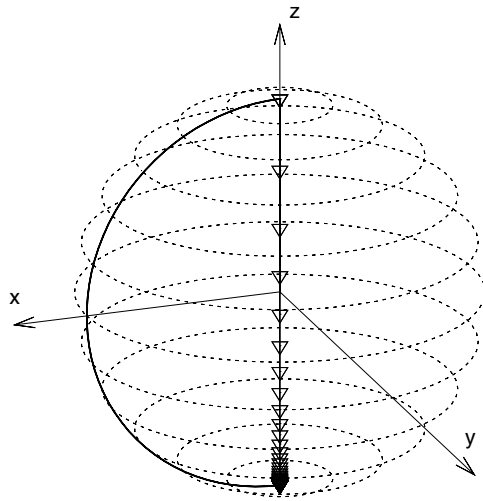
Figure 1. Analytical, time optimal evolution of $\rho(t)$ (arrows) in the Bloch sphere for the case of $r \times s = o$, $r \propto e_z$, $\gamma_1 = 0$, $\gamma_2 \neq 0$ and $\rho(0) = |\uparrow\rangle\langle\uparrow|$. Also shown (thick solid meridian curve) the optimal pure state evolution between the north and south poles (paper I).

Figure 2. Time optimal evolutions of a mixed state governed by the master equation with the Lindblad operators having magnitudes $\gamma_1 = \gamma_3 = 0$ and $\gamma_2 \neq 0$. Curves starting from $r = 0.8e_z$ and approaching $r = -e_z$ 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 r and s, i.e. $r \cdot s = rs \cos \frac{n\pi}{6}$, $n = 0, 1, \ldots, 5$.

5. A model for measurement or decoherence

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 (*A*) and the other is an externally controllable ancilla (*B*). The extra ancilla spin can be regarded as representing either a measurement apparatus or an environment. The two-qubit Hamiltonian can be chosen without loss of generality (modulo local rotations of the system and ancilla qubits) as

$$H_{AB}(t) := \sum_{j,k=x,y,z} h_{jk}(t)\sigma_j \otimes \sigma_k, \tag{32}$$

with time-dependent, tunable couplings $h_{jk}(t)$.[12]

The main goal of this section will be now to demonstrate how the optimal Hamiltonian and Lindblad operators found in the one-qubit model of the previous section can be actually simulated via the repetition of short time Markovian transitions in this simple two-qubit system by tuning the couplings in (32) and the state of the ancilla. In fact, the state of the system is described by the density operator (14) and the state of the ancilla by

$$\rho_B(t) := \tfrac{1}{2}[\mathbb{1} + \boldsymbol{b}(t) \cdot \boldsymbol{\sigma}], \tag{33}$$

where $\boldsymbol{b}$ is a tunable Bloch vector. The master equation in the Lindblad form (1) comes from the repetition of the unitary evolution by the interaction H_{AB} for a short time duration ε (i.e., for ε much smaller than the typical dynamical timescale of $\rho(t)$) and the partial trace over the *B* state. Namely,

$$\rho(t + \varepsilon) = \mathrm{Tr}_B\big[e^{-iH_{AB}\varepsilon}\rho(t) \otimes \rho_B(t)\, e^{iH_{AB}\varepsilon}\big]$$

$$= \rho(t) - i\varepsilon\, \mathrm{Tr}_B[H_{AB}, \rho(t) \otimes \rho_B(t)] + \varepsilon^2\big\{\mathrm{Tr}_B[H_{AB}(\rho(t) \otimes \rho_B(t))H_{AB}]$$

$$- \mathrm{Tr}_B\big[\tfrac{1}{2}\big\{H_{AB}^2, \rho(t) \otimes \rho_B(t)\big\}\big]\big\} + \mathcal{O}(\varepsilon^3). \tag{34}$$

For our model Hamiltonian, we can perform the partial trace over the *B* state and get

$$\rho(t + \varepsilon) = \rho(t) - i\varepsilon[H, \rho(t)]$$

$$+ \varepsilon^2 \sum_{j,k=x,y,z} a_{jk}(t)\bigg[\sigma_j\rho(t)\sigma_k - \frac{1}{2}\{\sigma_k\sigma_j, \rho(t)\}\bigg] + \mathcal{O}(\varepsilon^3), \tag{35}$$

where the effective single qubit Hamiltonian H is given in terms of the couplings h_{jk} and the Bloch vector b_j as

$$H(t) := \sum_{j,k=x,y,z} h_{jk}b_k\sigma_j, \tag{36}$$

while the Lindblad matrix is defined by

$$a_{jk}(t) := \sum_{l,m=x,y,z} h_{jl}h_{km}\bigg(\delta_{lm} - i\sum_{n=x,y,z}\epsilon_{lmn}b_n\bigg). \tag{37}$$

The eigenvectors and the eigenvalues of (37) together define the components of the Lindblad operators. Therefore, since the same components are also the eigenvectors in (21), one has to impose the commutativity condition $[a, K] = 0$, where K is given by (22). The real and imaginary parts of the later condition give three and nine constraints, respectively, so that we have twelve constraints in total for the nine parameters of h_{jk} and the three parameters of b_j. Then we can adjust the Hamiltonian couplings h_{jk} and the components b_j of the Bloch

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[12] For example, a tunable spin-spin coupling can be physically realized through superconducting flux qubits [30].

vector of the ancilla state so that the optimal $r(t)$, $s(t)$, $h(t)$ and $l_a(t)$ obtained in the previous section are reproduced.

In particular, if r and 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_{jk} as

$$(h_{jk}) = \begin{bmatrix} 0 & p & 0 \\ p & 0 & 0 \\ 0 & 0 & q \end{bmatrix}, \tag{38}$$

with real numbers p, q, and the Bloch vector b as

$$b = b e_z. \tag{39}$$

The Lindblad matrix (37) becomes

$$(a_{jk}) = \begin{bmatrix} p^2 & ibp^2 & 0 \\ -ibp^2 & p^2 & 0 \\ 0 & 0 & q^2 \end{bmatrix}. \tag{40}$$

Then the K matrix (26) for $\theta = 0$,

$$(K_{jk}) = 2s \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & r \end{bmatrix}, \tag{41}$$

and the Lindblad matrix a can be diagonalized simultaneously. In particular, the eigenvalues of a are $p^2(1 \mp b)$, q^2 and the corresponding eigenvectors are given as in (27)–(29), with the magnitudes of the Lindblad operators

$$\gamma_1^2 = (1 - b)\varepsilon p^2, \tag{42}$$

$$\gamma_2^2 = (1 + b)\varepsilon p^2, \tag{43}$$

$$\gamma_3^2 = \varepsilon q^2. \tag{44}$$

The optimal solution for $r(t)$ can be finally cast in the form

$$r(t) = [-b + (r(0) + b)\, e^{-4p^2\varepsilon t}]\, e_z. \tag{45}$$

An intuitive explanation for the behavior of the Bloch vector is the following. The exponential damping in (45) can be attributed to the standard formula for the transition probability calculated from the interaction Hamiltonian

$$H_{AB} = p(\sigma_x \otimes \sigma_y + \sigma_y \otimes \sigma_x) + q\sigma_z \otimes \sigma_z. \tag{46}$$

Note that q does not appear in (45) so that it can be put equal to zero. Suppose now that the B spin is up, i.e. $b = 1$. Since the interaction Hamiltonian (46) is proportional to $\sigma_+ \otimes \sigma_+ - \sigma_- \otimes \sigma_-$, both the system and the ancilla spins tend to align down. Suppose we start with the completely mixed state $r(0) = 0$. In the statistical interpretation of the density operator, this means that in half of the systems the spin is up while in the other half it is down. The up components are steered down while the down components remain unchanged, so that eventually the state of the system evolves from a completely mixed state to a purely down state. This kind of 'cooling' has been already discussed before [32]. On the other hand, for $b = 0$, the system approaches a completely mixed state regardless of the initial conditions, as we expect because the system is kept in contact with the completely random state of the ancilla, $\rho_B = \mathbb{1}/2$. This corresponds to decoherence. We would like to remark that although the coupling parameters h_{jk} and the ancilla state are constant in our particular parallel r and s case, they can be time dependent in general. This particular demonstration of a simple two-qubit model is enough to illustrate the physics behind the time-optimal evolution of a

one-qubit mixed state driven by a master equation in the Lindblad form which was presented in section 4.

6. Summary and discussion

We have developed a framework based on the variational principle for finding the time optimal quantum evolution necessary to steer the transition between given initial and final states ρ_i and ρ_f, when the physical system obeys a master equation in the Lindblad form. The equations of motion for the Hamiltonian H and the Lindblad operators 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 duration time T by solving the quantum brachistochrone together with the other equations of motion and imposing the initial and final conditions $\rho(0) = \rho_i$ and $\rho(T) = \rho_f$.

Our general formalism for the time optimal evolution of mixed states has been explicitly demonstrated with a one-qubit model. First, the optimal Hamiltonian was obtained from the quantum brachistochrone equation. Then the time evolution of the density operator and of the Lindblad operators which represent an optimal measurement or decoherence was found from a remaining set of ordinary differential and algebraic equations. In a particular case an analytical solution was given, while the solution for more general situations was shown numerically. To get a more physical intuition, we constructed an interacting two-qubit model where an ancilla qubit plays the role of the environment and we demonstrated that repeated short-time Markovian transitions can reproduce the time optimal evolution of mixed states.

It should be stressed here that although for the simplicity of the exposition we focused our attention on different implementations of the time optimal evolution of a one-qubit model, the general formalism of section 3 is valid for a Hilbert space of arbitrary finite dimensions. In particular, given the physical constraints on the Hamiltonian of a multiple-qubit open system, one can always find (albeit numerically) a solution to the quantum brachistochrone equation (12), obtain the optimal Hamiltonian and then, solving the remaining equations of motion (1), (7), (8) and (11), find the optimal Lindblad operators and the time-optimal quantum trajectory.

Our general formulation allows, in principle, the existence of time-dependent Lindblad operators. Master equations of the form (1) with an explicitly time-dependent Lindblad generator are known to be physically relevant for both the description of Markovian dynamics and the representation of non-Markovian time local dynamics in an extended Hilbert space (see, e.g., [24, 31]).

Our work has not dealt with the more general case of different duration times for the contacts between the system and the environment and the case of the possible memory feedback from the environment itself. The authors of [32] 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. Finally, 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 [33–35], we have not discussed this problem here.

Appendix. Gauge invariance of the master equation

The evolution of $\rho(t)$ described by the master equation (1) is invariant under the following gauge transformations [24, p 119],

$$H \mapsto H + u(t)\mathbb{1} + \frac{1}{2\mathrm{i}} \sum_a \left[v_a^*(t)L_a - v_a(t)L_a^\dagger \right],$$

$$L_a \mapsto L_a + v_a(t)\mathbb{1},$$
(A.1)

and

$$H \mapsto H, \qquad L_a \mapsto \sum_b U_{ab}(t)L_b,$$
(A.2)

where $u(t)$ is real, $v_a(t)$ 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 $u(t)$ in (A.1) corresponds to the $U(1)$ gauge degree of freedom which was discussed in papers I and II for the case of pure states. The gauge degrees of freedom $v_a(t)$, instead, correspond to the fact that the operator $H(t)$ in (1) is not just the free Hamiltonian of the reduced system, but may contain coupling terms with the environment (see, e.g., equation (36) in section 5). Finally, the $U_{ab}(t)$ represent the freedom of the choice of the basis for the Hilbert space of the environment.

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