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Time Optimal Quantum Evolution Within a Given Fidelity Range

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In a series of previous works we formulated a variational principle to find out the time-optimal evolution for a quantum system with a given set of initial and final states. Here we show how to obtain the shortest duration time $T(f)$ to reach the target state via quantum operations within a given fidelity larger than a specified value $f \leq 1$.

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I. INTRODUCTION

In a series of papers [1] we have considered the problem of finding the time-optimal path for the evolution of a quantum state and the optimal quantum operation with a driving Hamiltonian and measurements on the basis of variational principle. Before our work, Alvarez and Gómez [2] showed that the quantum state in Grover's algorithm [3], known as the optimal quantum search algorithm [4], actually follows a geodesic curve derived from the Fubini-Study metric in the projective space. Khaneja *et al.* [5] and Zhang *et al.* [6], using a Cartan decomposition scheme for unitary operations, discussed the time optimal way to realize a two-qubit universal unitary gate under the condition that one-qubit operations can be performed in an arbitrarily short time. On the other hand, Tanimura *et al.* [7] gave an adiabatic solution to the optimal control problem in holonomic quantum computation, in which a desired unitary gate is generated as the holonomy corresponding to the minimal length loop in the space of control parameters for the Hamiltonian. Schulte-Herbrüggen *et al.* [8] exploited the differential geometry of the projective unitary group to give the tightest known upper bounds on the actual time complexity of some basic modules of quantum algorithms. More recently, Nielsen [9] introduced a lower bound on the size of the quantum circuit necessary to realize a given unitary operator based on the geodesic distance, with a suitable metric, between the unitary and the identity operators.

In our previous work [1] we formulated the variational principle for the time-optimal evolution of a quantum system with a given set of initial and final states. However, it is more realistic to think of reaching the target state within a tolerable error. In the present work we are going to find the shortest duration time $T(f)$ to achieve the target state by quantum operations within a given fidelity larger than a specified value $f \leq 1$.

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II. VARIATIONAL PRINCIPLE

Let us consider the optimization problem described in the previous section on the basis of variational principle. In our problem the quantum state $|\psi(t)\rangle$ and the Hamiltonian $H(t)$ are the dynamical variables with a fixed initial state $|\psi(0)\rangle = |\psi_i\rangle$ but keeping the final state $|\psi(T)\rangle$ free within a fixed fidelity range. The action is defined as

$$S(\psi, H, \phi, \lambda) = S_F + \int dt \Big[\langle\phi|\dot{\psi}\rangle + i\langle\phi|H|\psi\rangle + \text{c.c.} + \sum_a \lambda^a f_a(H) \Big] \tag{1}$$

where $S_F = \lambda(f^2 - |\langle\psi_f|\psi(T)\rangle|^2)$ (with the Lagrange multiplier $\lambda(t) \in \mathbb{R}$) ensures that the fidelity of the final state $|\psi(T)\rangle$ with the target state $|\psi_f\rangle$ is f. The overdot denotes differentiation with respect to the time t. We have chosen units in which Planck's constant $\hbar$ is equal to one.

The second term guarantees, through the Lagrange multiplier $|\phi(t)\rangle \in \mathcal{H}$, that $|\psi(t)\rangle$ and $H(t)$ satisfy the Schrödinger equation and that the squared norm $\langle\psi|\psi\rangle = 1$ is conserved. The third term, through the Lagrange multipliers λ^a, generates a constraint for the Hamiltonian. The constraints correspond to the fact that physically only a finite amount of resources (e.g., a finite magnetic field) is available, and that only certain operations may be allowed (e.g., the magnetic field points in a definite direction).

Let us now derive the equations of motion. The variation of (1) with respect to $\langle\phi|$ leads to the Schrödinger equation

$$i|\dot{\psi}\rangle = H|\psi\rangle. \tag{2}$$

The variation with respect to $\langle\psi(t)|$, $t < T$ also produces the Schrödinger equation. The variation with respect to the end point $\langle\psi(T)|$, gives via the partial integration

$$|\phi(T)\rangle = \lambda\langle\psi_f|\psi(T)\rangle|\psi_f\rangle. \tag{3}$$

Finally, the variation with respect to the Hamiltonian H

is

$$F := \sum_a \lambda^a \frac{\partial f_a(H)}{\partial H} = -i[|\psi\rangle\langle\phi| - |\phi\rangle\langle\psi|]. \quad (4)$$

Equation (4) is an integrated version of the fundamental equation that we studied in the previous works. The problem reduces to solving the equations (4) together with the Schrödinger equations for $|\psi\rangle$ and $|\phi\rangle$ with the initial and final values, $|\psi(0)\rangle = |\psi_i\rangle$ and $|\phi(T)\rangle \propto |\psi_f\rangle$, respectively.

To be more specific we study quadratic and linear constraints,

$$f_0(H) := \mathrm{Tr}\, H^2/2 - \omega^2 = 0, \quad (5)$$
$$f_a(H) := \mathrm{Tr}(H\sigma_a) = 0, \quad (6)$$

where σ_a are subset of generators of $su(N)$ with normalization $Tr(\sigma_a\sigma_b) = 2\delta_{ab}$. We have

$$F = \lambda_0 H + \sum_a \lambda_a\sigma_a = -i[|\psi\rangle\langle\phi| - |\phi\rangle\langle\psi|]. \quad (7)$$

From the constraint $Tr(H\sigma_a) = 0$, we determine the Lagrange multipliers as

$$\lambda_a = \mathrm{Im}\langle\phi|\sigma_a\psi\rangle. \quad (8)$$

Choosing $\lambda_0 = 1$, we obtain the Hamiltonian

$$\begin{aligned} H &= -i[|\psi\rangle\langle\phi| - |\phi\rangle\langle\psi|] - \sum_a \mathrm{Im}\langle\phi|\sigma_a\psi\rangle\sigma_a \\ &= P(-i[|\psi\rangle\langle\phi| - |\phi\rangle\langle\psi|]) = \sum_a{}' \mathrm{Im}\langle\phi|\sigma'_a\psi\rangle\sigma'_a, \end{aligned} \quad (9)$$

where P stands for the projection to the space spanned by σ'_a orthogonal to σ_a. Palao and Kosloff [10] formulated a slightly restricted version of the variational principle for the optimal fidelity. They resorted to the numerical and iterative method to solve the Euler-Lagrange equation. We shall give a more formal development which enables us to access analytic solutions . Our formulation can also be viewed as the optimization of the fidelity with a fixed time duration.

III. A SIMPLE EXAMPLE

To illustrate the procedure consider the case that we have only the quadratic constraint. The Hamiltonian and the Schrödinger equations read,

$$\begin{aligned} |\dot\phi\rangle &= \langle\psi|\phi\rangle|\phi\rangle - \langle\phi|\phi\rangle|\psi\rangle \\ |\dot\psi\rangle &= |\phi\rangle - \langle\phi|\psi\rangle|\psi\rangle \end{aligned} \quad (10)$$

where we have used the normalization $\langle\psi|\psi\rangle = 1$ but keeping the normalization for $\langle\phi|\phi\rangle$ to be determined. Introducing the normalized state $|\tilde\phi\rangle = (|\phi\rangle - \langle\psi|\phi\rangle|\psi\rangle)/N$ orthogonal to $|\psi\rangle$ with $N := \sqrt{\langle\phi|\phi\rangle - \langle\phi|\psi\rangle\langle\psi|\phi\rangle}$ being the normalization. Then (10) simply becomes

$$\begin{aligned} |\dot{\tilde\phi}\rangle &= -N|\psi\rangle \\ |\dot\psi\rangle &= N|\tilde\phi\rangle, \end{aligned} \quad (11)$$

with the use of $\langle\psi|\phi\rangle = const = \langle\psi(T)|\phi(T)\rangle = \lambda f^2 \in \mathbb{R}$. The solution is

$$|\psi(t)\rangle = \cos Nt|\psi(0)\rangle + \sin Nt|\tilde\phi(0)\rangle. \quad (12)$$

The (constant) Hamiltonian then becomes

$$H = iN[|\tilde\phi\rangle\langle\psi| - |\psi\rangle\langle\tilde\phi|] \quad (13)$$

and the constraint (5) (we choose $\omega > 0$) gives $N = \omega$. Recalling that the fidelity f is defined by

$$\langle\psi_f|\psi(T)\rangle := fe^{i\zeta}, \quad (14)$$

with an arbitrary phase ζ, we then obtain

$$\begin{aligned} |\psi(t)\rangle = &\left(\cos\omega t - \frac{f}{\sqrt{1-f^2}}\sin\omega t\right)|\psi_i\rangle \\ &+ \frac{\sin\omega t e^{i\zeta}}{\sqrt{1-f^2}} e^{iHT}|\psi_f\rangle. \end{aligned} \quad (15)$$

Here we have used $\lambda = \omega/(f\sqrt{1-f^2})$ and

$$\begin{aligned} H &= i\omega[|\tilde\phi\rangle\langle\psi| - |\psi\rangle\langle\tilde\phi|] \\ e^{iHT} &= \cos\omega T - \sin\omega T[|\tilde\phi\rangle\langle\psi| - |\psi\rangle\langle\tilde\phi|] \\ \langle\psi_f|e^{iHT}\psi_f\rangle &= \cos\omega T \\ \langle\psi_f|\tilde\phi(T)\rangle &= \sqrt{1-f^2}e^{i\zeta} \\ \langle\psi(T)|\phi(T)\rangle &= \omega\frac{f}{\sqrt{1-f^2}} \end{aligned} \quad (16)$$

Let us find out the duration time T by

$$\begin{aligned} f = &\left(\cos\omega T - \sin\omega T\frac{f}{\sqrt{1-f^2}}\right)\langle\psi_f|\psi_i\rangle e^{-i\zeta} \\ &+ \frac{\sin\omega T\cos\omega T}{\sqrt{1-f^2}}. \end{aligned} \quad (17)$$

The imaginary part of this equation gives $e^{-i\zeta} = \pm 1$ so that we obtain either $\omega T = \chi + n\pi,\ n \in Z$ or

$$\omega T = \theta - \chi + m\pi,\ m \in Z \quad (18)$$

with $\langle\psi_f|\psi_i\rangle := \cos\theta$ and $f := \cos\chi$. In particular, if $|\psi_f\rangle$ and $|\psi_i\rangle$ are orthogonal, i.e. $\theta = \pi/2$, the duration time is given by $\omega T = \pi/2 - \chi$ and (18) can be geometrically understood if we consider a great circle and the angles corresponding to the target state θ and the fidelity allowance χ.

IV. A SINGLE QUBIT EXAMPLE WITH THE TWO CONSTRAINTS

Now let us take into account the linear constraint $Tr(H\sigma_z) = 0$. On the basis of the general discussion before, we see that the Hamiltonian is

$$\begin{aligned} H &= X\sigma_x + Y\sigma_y, \\ X &= \mathrm{Im}[\langle\phi|\sigma_x\psi\rangle] \\ Y &= \mathrm{Im}[\langle\phi|\sigma_y\psi\rangle], \\ Z &= \mathrm{Im}[\langle\phi|\sigma_z\psi\rangle]. \end{aligned} \tag{19}$$

X satisfies the differential equation,

$$\begin{aligned} \dot{X} &= \mathrm{Im}[\langle\dot{\phi}|\sigma_x\psi\rangle + \langle\phi|\sigma_x\dot{\psi}\rangle]] \\ &= \mathrm{Im}[i\langle\phi|[H,\sigma_x]\psi\rangle] \\ &= 2YZ. \end{aligned} \tag{20}$$

Similarly we have

$$\begin{aligned} \dot{Y} &= -2XZ, \\ \dot{Z} &= 0. \end{aligned} \tag{21}$$

The initial condition $(1-P_i)F(0)(1-P_i) = 0$, with $P_i := |\psi_i\rangle\langle\psi_i|$ fixes the initial value of X equal to zero so that we get the solution writing $Z = \Omega = const.$,

$$\begin{aligned} X &= \omega\sin(2\Omega t), \\ Y &= \omega\cos(2\Omega t), \end{aligned} \tag{22}$$

where we have used the quadratic constraint $Tr(H^2) = 2\omega^2$. The Hamiltonian can be rewritten as

$$H(t) = \omega e^{i\Omega t\sigma_z}\sigma_y e^{-i\Omega t\sigma_z} \tag{23}$$

Let $|\psi\rangle = e^{i\Omega t\sigma_z}|\tilde{\psi}\rangle$ to reduce the Schrödinger equation to

$$i|\dot{\tilde{\psi}}\rangle = (\Omega\sigma_z + \omega\sigma_y)|\tilde{\psi}\rangle := \Omega'\tilde{\sigma}|\tilde{\psi}\rangle, \tag{24}$$

where $\Omega' := \sqrt{\Omega^2+\omega^2}$ and $\tilde{\sigma} := (\Omega\sigma_z + \omega\sigma_x/\Omega'$.

The solution is

$$|\tilde{\psi}(t)\rangle = e^{-i\Omega'\tilde{\sigma}t}|\tilde{\psi}(0)\rangle \tag{25}$$

so that

$$|\psi(t)\rangle = U(t)|\psi(0)\rangle = e^{i\Omega t\sigma_z}e^{-i\Omega'\tilde{\sigma}t}|\psi_i\rangle. \tag{26}$$

More explicitly

$$U(t) = e^{i\Omega t\sigma_z}e^{-i\Omega'\tilde{\sigma}t} \tag{27}$$

$$= \cos\Omega t\cos\Omega' t + \frac{\Omega}{\Omega'}\sin\Omega t\sin\Omega' t \tag{28}$$

$$+ i\Big[-\frac{\omega}{\Omega'}(\sin\Omega t\sin\Omega' t\sigma_x + \cos\Omega t\sin\Omega' t\sigma_y) \tag{29}$$

$$+ (\sin\Omega t\cos\Omega' t - \frac{\Omega}{\Omega'}\cos\Omega t\sin\Omega' t)\sigma_z\Big] \tag{30}$$

We are now going to determine the three integration constants Ω, T and λ by the four equations

$$\begin{aligned} f^2 &= |\langle\psi_f|\psi(T)\rangle|^2, \\ X(T) &= \omega\sin 2\Omega T = \mathrm{Im}[\langle\phi(T)|\sigma_x\psi(T)\rangle], \\ Y(T) &= \omega\cos 2\Omega T = \mathrm{Im}[\langle\phi(T)|\sigma_y\psi(T)\rangle], \\ Z(T) &= \Omega = \mathrm{Im}[\langle\phi(T)|\sigma_z\psi(T)\rangle], \end{aligned} \tag{31}$$

one of which is redundant. Here $|\phi(T)\rangle$ is related to the target state $|\psi_f\rangle$ by (3). The above set of equations can be solved for Ω, T and λ once the target state $|\psi_f\rangle$ and the required fidelity are given. In the following we illustrate the procedure for the special choice of $|\psi_i\rangle$ and $|\psi_f\rangle$,which is a slight generalization of the one in the paper 1[1].

$$|\psi_i\rangle = \frac{(1,1)}{\sqrt{2}} \tag{32}$$

$$|\psi_f\rangle = \frac{(e^{i\theta}, e^{-i\theta})}{\sqrt{2}}. \tag{33}$$

Namely,we consider an optimal unitary transition from a state to another on the equator within a given fidelity f in the Bloch sphere. A straightfoward calculation gives

$$\begin{aligned} X &= \mathrm{Im}[\langle\phi(T)|\sigma_x\psi(T)\rangle] \\ &= \lambda\ \mathrm{Im}[\langle\psi_f|\psi(T)\rangle^*\langle\psi_f|\sigma_x\psi(T)\rangle] \\ &= \lambda\ \mathrm{Im}\bigg(\Big[\cos(\Omega T-\theta)\cos\Omega' T + \frac{\Omega}{\Omega'}\sin(\Omega T-\theta)\sin\Omega' T \\ &+ i\frac{\omega}{\Omega'}\sin(\Omega T-\theta)\sin\Omega' T\Big]\Big[\cos(\Omega T+\theta)\cos\Omega' T \\ &+ \frac{\Omega}{\Omega'}\sin(\Omega T+\theta)\sin\Omega' T + i\frac{\omega}{\Omega'}\sin(\Omega T+\theta)\sin\Omega' T\Big]\bigg) \\ &= -\frac{\omega\lambda}{2\Omega'}\sin 2\theta\sin 2\Omega' T \end{aligned} \tag{34}$$

Similarly we have

$$\begin{aligned} Y &= -\frac{\omega\lambda}{2\Omega'}\cos 2\theta\sin 2\Omega' T \\ Z &= \frac{\lambda}{2}\Big[\sin(2\Omega T-2\theta)\cos 2\Omega' T \\ &- \frac{\Omega}{\Omega'}\cos(2\Omega T-2\theta)\sin 2\Omega' T\Big] \\ 2f^2-1 &= \cos(2\Omega T-2\theta)\cos 2\Omega' T \\ &+ \frac{\Omega}{\Omega'}\sin(2\Omega T-2\theta)\sin 2\Omega' T \end{aligned} \tag{35}$$

The last equation comes from the definition of fidelity $f^2 = |\langle\psi_f|\psi(T)\rangle|^2$. From (34) and (35) we see that

$$\lambda = -\frac{2\Omega'}{\sin 2\Omega' T} \tag{36}$$

Then the solutions of $X = \omega\sin\Omega T$ and $Y = \omega\cos\Omega T$ imply

$$\Omega T = \theta - \frac{\pi}{2} + n\pi,\ n \in Z, \tag{37}$$

the equation for Ω is automatically satisfied and the last equation for the fidelity $2f^2 - 1 = \cos 2\Omega' T$ gives

$$\Omega' T = \frac{1}{2}\arccos(1 - 2f^2) + \pi + n\pi,\ m \in Z. \qquad (38)$$

Combining (37)and(38) we finally arrive at the expression for the duration time T

$$\omega T = \sqrt{(\pi/2 - \chi + n\pi)^2 - (\pi/2 - \theta + m\pi)^2},\ m, n \in Z, \qquad (39)$$

where the fidelity angle χ is defined by $f = \cos\chi$. It is curious to point out that the obtained minimum duration time $\omega T_{MIN} = \sqrt{(\pi/2 - \chi)^2 - (\pi/2 - \theta)^2} = \sqrt{(\theta - \chi)(\pi - \theta - \chi)}$ is the geometric mean of the minimum time and maximum time along the equator to the target region. To conclude this section we just present the trajectory in the Bloch sphere

$$\begin{aligned} x(t) &= \langle\psi(t)|\sigma_x\psi(t)\rangle = \cos 2\Omega t \cos 2\Omega' t \\ &+ \frac{\Omega}{\Omega'}\sin 2\Omega t \sin 2\Omega' t, \\ y(t) &= \langle\psi(t)|\sigma_y\psi(t)\rangle = -\sin 2\Omega t \cos 2\Omega' t \\ &+ \frac{\Omega}{\Omega'}\cos 2\Omega t \sin 2\Omega' t, \\ z(t) &= \langle\psi(t)|\sigma_z\psi(t)\rangle = -\frac{\omega}{\Omega'}\sin 2\Omega' t. \end{aligned} \qquad (40)$$

for the minimum duration time. The other local minima for various $m, n \in Z$ can be easily obtained.

V. SUMMARY

We have formulated a variational principle to obtain the time-optimal evolution for a quantum system to reach the target state with the shortest duration time $T(f)$ and within a given fidelity larger than a specified value $f \le 1$. One qubit examples are demonstrated to show simple geometric interpretations. We hope the present approach is helpful to develop a fast approximate quantum algorithm.

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