Time-Optimal Quantum Evolution

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We present a general framework for finding the time-optimal evolution and the optimal Hamiltonian for a quantum system with a given set of initial and final states. Our formulation is based on the variational principle and is analogous to that for the brachistochrone in classical mechanics. We reduce the problem to a formal equation for the Hamiltonian which depends on certain constraint functions specifying the range of available Hamiltonians. For some simple examples of the constraints, we explicitly find the optimal solutions.

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In quantum mechanics one can change a given state to another by applying a suitable Hamiltonian on the system. In many situations, e.g., quantum computation, it is desirable to know the pathway in the shortest time.

In this Letter we consider the problem of finding the time-optimal path for the evolution of a pure quantum state and the optimal driving Hamiltonian. Recently, a growing number of works related to this topic have appeared. For instance, Alvarez and Gómez [1] showed that the quantum state in Grover's algorithm [2], known as the optimal quantum search algorithm [3], actually follows a geodesic curve derived from the Fubini-Study metric in the projective space. Khaneja *et al.* [4] and Zhang *et al.* [5], 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.* [6] 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.* [7] 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 [8] 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. However, a general method for generating the time-optimal Hamiltonian evolution of quantum states was not known until now.

Here we are going to study this problem by exploiting the analogy with the so-called brachistochrone problem in classical mechanics and the elementary properties of quantum mechanics. In ordinary quantum mechanics the initial state and the Hamiltonian of a physical system are given and one has to find the final state using the Schrödinger equation. In our work we generalize this framework so as to optimize a certain cost functional with respect to the Hamiltonian as well as the quantum states. The cost functional quantifies the efficiency to get the target state from a given initial state and depends on the physical situation. In this Letter we focus our attention on the time optimality but it is straightforward to generalize our methods to other cost functions.

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

Let us now move to the time optimization problem in the quantum case. We want to minimize the total amount of time necessary for changing a given initial state $|\psi_i\rangle$ (belonging to an n-dimensional Hilbert space $\mathcal{H}$) to a given final state $|\psi_f\rangle$, by suitable choice of a (possibly time-dependent) Hamiltonian $H(t)$. In our problem the quantum state $|\psi(t)\rangle$ and the Hamiltonian $H(t)$ are the dynamical variables, and the action is defined as

$$S(\psi, H, \phi, \lambda) = \int dt \Bigg[\frac{\sqrt{\langle \frac{d}{dt}\psi|(1-P)|\frac{d}{dt}\psi\rangle}}{\Delta E} + (i\langle \tfrac{d}{dt}\phi|\psi\rangle + \langle\phi|H|\psi\rangle + \text{c.c.}) + \lambda\bigg(\frac{\text{Tr}\tilde{H}^2}{2} - \omega^2\bigg)\Bigg]. \quad (1)$$

Here $P(t) := |\psi(t)\rangle\langle\psi(t)|$ is the projection to the state $|\psi(t)\rangle$, $\tilde{H} := H - (\text{Tr}H)/n$ is the traceless part of the Hamiltonian, $(\Delta E)^2 := \langle\psi|H^2|\psi\rangle - \langle\psi|H|\psi\rangle^2$ is the energy variance, and ω is a given nonzero constant. To simplify the notation we write $\frac{d}{dt}|\psi\rangle$ as $|\frac{d}{dt}\psi\rangle$ and so forth.

We have chosen units in which Planck's constant $\hbar$ is equal to one.

The first term in the action (1) gives the time duration for the evolution of $|\psi(t)\rangle$, expressed in terms of the Fubini-Study line element $ds^2 = \langle d\psi|(1-P)|d\psi\rangle$ on the projective space $\mathbb{C}P^{n-1}$. 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 multiplier λ, generates a constraint for the Hamiltonian. Such a constraint is necessary because otherwise one would be able to find a path with arbitrarily small time duration just by rescaling the Hamiltonian as $H \mapsto \alpha H$, with $\alpha > 1$, to make the energy fluctuations ΔE large. This corresponds to the fact that physically only a finite amount of resources (e.g., a finite magnetic field) is available. Here we consider a typical example which we call the isotropic constraint (we will consider more general constraints later). The constraint is imposed on $\tilde{H}$ rather than H, since the difference between the highest and the lowest energy levels in H, and not the value of the energy levels themselves, is important for the physical system. The problem should be mathematically formulated on the projective space $\mathbb{C}P^{n-1}$ rather than on $\mathcal{H}$, because the overall phase of the state $|\psi\rangle$ is of no significance in quantum mechanics. In fact, the action (1) is invariant under the $U(1)$ gauge transformation $(|\psi\rangle, H, |\phi\rangle, \lambda) \mapsto (e^{-i\theta}|\psi\rangle, H + \frac{d\theta}{dt}, e^{-i\theta}|\phi\rangle, \lambda)$, where $\theta(t)$ is a real function. Note that the Hamiltonian H plays the role of the gauge potential (there is also another symmetry, $|\phi\rangle \mapsto |\phi\rangle + i\gamma|\psi\rangle$, where γ is a real constant).

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

$$i\frac{d}{dt}|\psi\rangle = H|\psi\rangle. \tag{2}$$

In particular, this implies $\langle \frac{d}{dt}\psi|(1-P)|\frac{d}{dt}\psi\rangle = (\Delta E)^2$, or

$$ds = \Delta E dt, \tag{3}$$

which was found by Aharonov and Anandan [9] and leads to a rigorous formulation of the time-energy uncertainty principle. The variation with respect to λ gives the constraint $\mathrm{Tr}\tilde{H}^2 = 2\omega^2$. The variation with respect to $\langle\psi|$, upon using (2), yields

$$i\left[\frac{d}{dt}\left(\frac{H - \langle H\rangle}{2(\Delta E)^2}\right)\right]|\psi\rangle - i\frac{d}{dt}|\phi\rangle + H|\phi\rangle = 0. \tag{4}$$

Finally, the variation with respect to H, after use of (2), implies

$$\frac{\{H, P\} - 2\langle H\rangle P}{2(\Delta E)^2} - \lambda\tilde{H} - (|\psi\rangle\langle\phi| + |\phi\rangle\langle\psi|) = 0, \tag{5}$$

where a bracket $\langle\bullet\rangle$ denotes the expectation value with respect to $|\psi\rangle$ and $\{A, B\} = AB + BA$. Equation (4) and the trace of (5) imply that $\langle\psi|\phi\rangle$ is a purely imaginary constant. Then, the expectation value of (5) gives $\langle\tilde{H}\rangle = 0$, which is equivalent to $\langle H\rangle = (\mathrm{Tr}H)/n$, or $\tilde{H} = H - \langle H\rangle$. Applying (5) to $|\psi\rangle$, we have

$$|\phi\rangle = \left[\left(\frac{1}{2(\Delta E)^2} - \lambda\right)\tilde{H} + \langle\psi|\phi\rangle\right]|\psi\rangle, \tag{6}$$

and inserting (6) back into (5), we obtain

$$\tilde{H} = \tilde{H}P + P\tilde{H}. \tag{7}$$

Furthermore, the energy variance is constant; i.e., $(\Delta E)^2 = \langle\tilde{H}^2\rangle = \mathrm{Tr}\tilde{H}^2/2 = \omega^2$. Substituting (6) into (4), we have $\frac{d(\lambda\tilde{H})}{dt}|\psi\rangle = 0$ which, after multiplication by $\langle\psi|H$, implies that λ is constant. We then obtain

$$\frac{d\tilde{H}}{dt}|\tilde{\psi}\rangle = 0, \tag{8}$$

where we have introduced $|\tilde{\psi}\rangle := \exp[i\int_0^t\langle H\rangle dt]|\psi\rangle$. In conclusion, the equations to be solved have reduced to (7) and (8). Equation (7) gives an expression for the optimal Hamiltonian and (8) gives the optimal time evolution of the quantum state. In fact, the state $|\tilde{\psi}\rangle$ satisfies the Schrödinger equation with Hamiltonian $\tilde{H}$, and (7) implies

$$\tilde{H} = i(|\tfrac{d}{dt}\tilde{\psi}\rangle\langle\tilde{\psi}| - |\tilde{\psi}\rangle\langle\tfrac{d}{dt}\tilde{\psi}|). \tag{9}$$

The derivative $|\frac{d}{dt}\tilde{\psi}\rangle$ is orthogonal to $|\tilde{\psi}\rangle$ because $\langle\tilde{H}\rangle = 0$. Therefore, Eq. (8) reads

$$(1 - \tilde{P})\frac{d^2}{dt^2}|\tilde{\psi}\rangle = 0, \tag{10}$$

where $\tilde{P} = |\tilde{\psi}\rangle\langle\tilde{\psi}| = P$. This is the geodesic equation for the Fubini-Study metric on $\mathbb{C}P^{n-1}$, which is suggested by the observation that the first term in the action (1) becomes $\int ds$ for constant ΔE. We also easily see that $\frac{d}{dt}\tilde{H} = 0$ from (9) and (10).

One can solve Eq. (10) using $(\Delta E)^2 = \omega^2$, finding:

$$|\tilde{\psi}(t)\rangle = \cos\omega t|\tilde{\psi}(0)\rangle + \frac{\sin\omega t}{\omega}|\tfrac{d}{dt}\tilde{\psi}(0)\rangle. \tag{11}$$

It is then easy to rewrite (11) and $\tilde{H}$ in terms of the Gram-Schmidt orthonormalized initial state $|\psi_i\rangle$ and final state $|\psi_f'\rangle$ as

$$|\tilde{\psi}(t)\rangle = \cos\omega t|\psi_i\rangle + \sin\omega t|\psi_f'\rangle, \tag{12}$$

$$\tilde{H} = i\omega(|\psi_f'\rangle\langle\psi_i| - |\psi_i\rangle\langle\psi_f'|). \tag{13}$$

As a result, the whole Hamiltonian is given by $H(t) = \tilde{H} + \langle H(t)\rangle$, where $\langle H(t)\rangle$ is an arbitrary real function corresponding to the gauge degree of freedom. The optimal time is $T = \frac{1}{|\omega|}\arccos|\langle\psi_f|\psi_i\rangle|$.

Let us now generalize the quantum brachistochrone problem to the case of a more general set of m constraints for the Hamiltonian $H(t)$. This extension is of relevance, for example, when some operations are not implementable in practice. Instead of (1) we consider the action

$$S(\psi, H, \lambda, \mu) = \int dt\left[\frac{\sqrt{\langle \frac{d}{dt}\psi|(1-P)|\frac{d}{dt}\psi\rangle}}{\Delta E} + (i\langle \tfrac{d}{dt}\phi|\psi\rangle + \langle\phi|H|\psi\rangle + \text{c.c.}) + \sum_{a=1}^{m}\lambda^a f_a(H)\right], \tag{14}$$

where the f_a $(a = 1, \ldots m)$ are functions mapping a Hermitian operator into a real number. As we have already discussed, the most natural case to consider is when the f_a are actually functions of $\tilde{H}$, but the argument below is also valid for arbitrary f_a. Among the equations of motion, the constraint now generalizes to $f_a(H) = 0$, while (7) and (8) become

$$F = FP + PF, \tag{15}$$

$$\left(\frac{dF}{dt} + i[\tilde{H}, F]\right)|\psi\rangle = 0, \tag{16}$$

with the operator

$$F(H) := \sum_a \lambda^a\left(\frac{\delta f_a}{\delta H} - \left\langle\frac{\delta f_a}{\delta H}\right\rangle P\right). \tag{17}$$

In particular, Eq. (15) guarantees that $\mathrm{Tr}F = \langle F\rangle = 0$. Note that, for $m = 1$ and $f = \mathrm{Tr}\tilde{H}^2/2 - \omega^2$, Eqs. (15) and (16) reproduce (7) and (8) of the isotropic case.

We can formally integrate (15) and (16) to obtain

$$F = UF(0)U^\dagger, \tag{18}$$

where $F(0)$ is a constant Hermitian operator which satisfies $F(0) = \{F(0), P(0)\}$ and the unitary operator U is given as a functional of $\tilde{H}$,

$$U[\tilde{H}](t) := \hat{T}e^{-i\int_0^t \tilde{H}dt}, \tag{19}$$

with $\hat{T}$ the time-ordered product. Thus, given the constraints $f_a(\tilde{H}) = 0$, one can explicitly write the left hand side of (18) as a function of $\tilde{H}$ and solve (18) to obtain the optimal Hamiltonian $\tilde{H}$. This is our main result.

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

$$f_1(H) := \mathrm{Tr}\tilde{H}^2/2 - \omega^2 = 0, \tag{20}$$

$$f_2(H) := \mathrm{Tr}(\tilde{H}\sigma_z) = 0, \tag{21}$$

where σ_j $(j = x, y, z)$ are the Pauli matrices. Note that for the one-qubit system the traceless Hamiltonian can be written in general as $\tilde{H}(t) = -\boldsymbol{\sigma}\cdot\boldsymbol{B}(t)$, with $\boldsymbol{B} \in \mathbb{R}^3$. The constraints (20) and (21) imply that $|\boldsymbol{B}| = |\omega|$ and $\boldsymbol{B} = (B_x, B_y, 0)$. This corresponds to, e.g., the physical system of a spin-1/2 particle with unit magnetic moment in a magnetic field $\boldsymbol{B}$. The spin is controlled by the magnetic field of magnitude given by the Larmor frequency ω and with x and y components only. By (18) and $\mathrm{Tr}F = 0$, we have

$$F = \lambda_1\tilde{H} + \lambda_2\sigma_z = UF(0)U^\dagger. \tag{22}$$

Eliminating $\tilde{H}$ in (22) via $i\frac{d}{dt}U = \tilde{H}U$ and solving (22), we get $U = \exp[i\chi\sigma_z]\exp[-iF(0)\int_0^t dt/\lambda_1]$, where $\chi(t) := \int_0^t(\lambda_2/\lambda_1)dt$. From (20)–(22) and the above formula for U, we find that the λ_j are constants and we can simplify U and $\tilde{H}$ as

$$U = e^{i\Omega t\sigma_z}e^{-i[\tilde{H}(0)+\Omega\sigma_z]t}, \tag{23}$$

$$\tilde{H} = e^{i\Omega t\sigma_z}\tilde{H}(0)e^{-i\Omega t\sigma_z}, \tag{24}$$

where $\Omega := \lambda_2/\lambda_1$.

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 towards the positive x direction. Then the condition $F(0) = \{F(0), P(0)\}$ and the constraints (20) and (21) imply that $\tilde{H}(0) = -\omega\sigma_y$, and from (23) and (24) we finally obtain

$$\langle\boldsymbol{\sigma}\rangle(t) = \begin{pmatrix} \cos2\Omega t\cos2\Omega' t + \frac{\Omega}{\Omega'}\sin2\Omega t\sin2\Omega' t \\ -\sin2\Omega t\cos2\Omega' t + \frac{\Omega}{\Omega'}\cos2\Omega t\sin2\Omega' t \\ \frac{\omega}{\Omega'}\sin2\Omega' t \end{pmatrix}, \tag{25}$$

$$\tilde{H}(t) = -\boldsymbol{\sigma}\cdot\boldsymbol{B}(t), \qquad \boldsymbol{B}(t) = \omega\begin{pmatrix}\sin2\Omega t\\ \cos2\Omega t\\ 0\end{pmatrix}, \tag{26}$$

where $\Omega' := \sqrt{\omega^2 + \Omega^2}$. We can interpret $\boldsymbol{B}(t)$ as a magnetic field rotating with angular velocity 2Ω. Equation (25) is not a geodesic on $\mathbb{C}P^1$ unless $\Omega = 0$, in which case the orbit is a great circle in the xz plane. The energy fluctuation (which is also the speed of the state) is now time dependent, $\Delta E(t) = |\omega|[1 - (\frac{\Omega}{\Omega'}\sin2\Omega' t)^2]^{1/2}$. We notice that the constraint (21) in general reduces the speed of the state.

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 $P(T) = (1 - \sigma_x)/2$, which is the antipodal point of $P(0)$ in $\mathbb{C}P^1$. Then we have the conditions $2|\Omega|T = k\pi$ and $2\Omega' T = l\pi$, where k and l are integers such that $l > k \geq 0$ and $k + l$ is odd. Thus we get

$$|\omega|T = \frac{\pi}{2}\sqrt{l^2 - k^2}, \qquad \left|\frac{\Omega}{\omega}\right| = \frac{k}{\sqrt{l^2 - k^2}}. \tag{27}$$

The concrete solutions for (27), in ascending order of T, are $(|\omega|T, |\frac{\Omega}{\omega}|) = (\frac{\pi}{2}, 0), (\frac{\pi}{2}\sqrt{3}, \frac{1}{\sqrt{3}}), (\frac{\pi}{2}\sqrt{5}, \frac{2}{\sqrt{5}}), \ldots$. These solutions, respectively, have zero, one, two,... nodes along the great circle $\langle\sigma_z\rangle = 0$. The first one is a geodesic, while the others are not. On the other hand, if the final state is not in the xz plane, there is no geodesic solution. At this stage

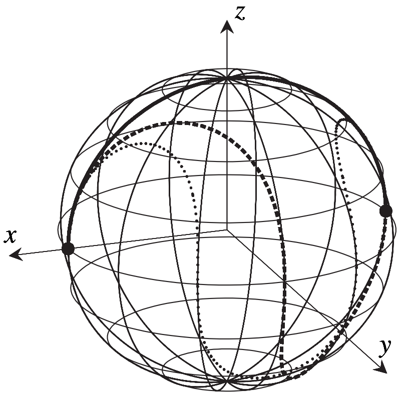

FIG. 1. Locally optimal curves on the Bloch sphere. The solid, thick dotted, and thin dotted curves correspond, respectively, to the solutions with $|\omega|T = \frac{\pi}{2}$, $\frac{\pi}{2}\sqrt{3}$, and $\frac{\pi}{2}\sqrt{5}$. They have zero, one, and two nodes along the great circle on the xy plane, respectively.

we have to caution the reader that solutions may be only locally optimal, and we have to find out the globally optimal one by comparing time durations T. In the above case, the first curve without nodes is globally optimal. The second curve becomes globally optimal if the final state is its first node. The solutions are depicted in Fig. 1.

In summary, in analogy to the classical brachistochrone problem we have formulated a variational principle to find the optimal Hamiltonian and the optimal quantum state evolution, for given initial and final states and a set of available Hamiltonians. As a particular application of our methods, one might want to first evaluate the optimal Hamiltonian, e.g., by means of a classical computer, and then perform the fastest possible quantum experiment or quantum computation. The classical computational complexity of (18) may be also an interesting problem to pursue. As a future development of the present research we do not see any obstacle to generalizing our formulation to mixed states. The relation to gate complexity in the standard paradigm of quantum computation remains to be investigated, though our point of view is that the time complexity (see, e.g., Schulte-Herbrüggen *et al.* [7] and references therein) is more physical or even more practical. For example, Eqs. (12) and (13) essentially solve Grover's search problem [1,2]. However, to show the square-root speed up with respect to the classical case one still has to identify the computational step corresponding to a single oracle call. We hope that the present variational approach to the time optimality problem in quantum mechanics opens up novel systematic investigations of optimal quantum computation.

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