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Quantum Brachistochrone Curves as Geodesics: Obtaining Accurate Minimum-Time Protocols for the Control of Quantum Systems

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Most methods of optimal control cannot obtain accurate time-optimal protocols. The quantum brachistochrone equation is an exception, and has the potential to provide accurate time-optimal protocols for a wide range of quantum control problems. So far, this potential has not been realized, however, due to the inadequacy of conventional numerical methods to solve it. Here we show that the quantum brachistochrone problem can be recast as that of finding geodesic paths in the space of unitary operators. We expect this brachistochrone-geodesic connection to have broad applications, as it opens up minimal-time control to the tools of geometry. As one such application, we use it to obtain a fast numerical method to solve the brachistochrone problem, and apply this method to two examples demonstrating its power.

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The ability to realize a prescribed evolution for a given physical quantum device is important in a range of applications. A powerful approach to this task is to vary the Hamiltonian of the device with time [1–3]. A prescription for a time-dependent Hamiltonian realizing a desired evolution is called a “control protocol,” and a protocol that achieves this task in the minimal time is called “time-optimal” [4,5]. Because the ever-present noise from the environment degrades quantum states over time, generating the fastest possible evolution is important in information processing [6–8], metrology [9–11], cooling [12,13], and experiments that probe quantum behavior [14–17]. Finding accurate time-optimal protocols is difficult because it is a two-objective optimization problem: one must minimize the error in the resulting evolution while simultaneously minimizing the time taken by the protocol (hereafter, the “protocol time”). Finding approximate protocols, on the other hand, is relatively easy: one can minimize a weighted sum of the two objectives [1], or search for protocols at a range of fixed times to locate a likely minimum time. But there is presently no practical way to refine these further. Analytical methods that use the Pontryagin maximum principle or the geometry of the unitary group are useful only for specific kinds of problems and constraints [5,18–26]. In view of this, the quantum brachistochrone equation (QBE) was a significant development [27–29]. It has the potential to provide accurate time-optimal protocols under two physically relevant constraints: (i) the system has a finite energy bandwidth (the norm of the Hamiltonian is bounded); and (ii) the Hamiltonian is restricted to a subspace

of Hermitian operators. Nevertheless, an obstacle remains that has prevented the QBE from becoming a practical tool: the QBE transforms the optimization problem into that of solving an ordinary differential equation (ODE) with boundary values, but there exists no numerical method that can solve such a boundary-value problem (BVP) efficiently in high dimensions. The available methods, namely “simple shooting,” “multiple shooting,” finite difference, and finite-element (or variational) methods [30], convert the BVP into a set of nonlinear algebraic equations which are then solved by a numerical search method (e.g., quasi-Newton or conjugate gradient methods [31]). These search methods fail unless provided with a sufficiently good initial guess. Even for systems as small as two qubits, a random guess is insufficient, with the result that the QBE has been solved only for special cases that possess analytic solutions [32–34].

Here we show that, under constraints (i) and (ii) above, the minimum-time control problem can be transformed into that of finding a shortest path—a geodesic—on a manifold. If we imagine driving a car over some smooth but undulating terrain, then if the speed of the car is bounded, and we can always travel at the maximum speed, the shortest time is achieved by the shortest route. We will see that, for quantum dynamics, the norm of the Hamiltonian is analogous to the speed of the car. Further, constraints of type (ii) in the brachistochrone can be included in the geodesic setting by choosing an appropriate norm. This provides a new, fully geometric interpretation of minimal-time problems. In fact, differential geometry has been

found to be important to study quantum computation and quantum control [4,35–37]. Our second primary result is an effective numerical method for solving the brachistochrone equation, obtained by exploiting the brachistochrone-geodesic connection.

Preliminaries.—To generate a target unitary V on an n -dimensional quantum system, we need to find a time-varying Hamiltonian $H(t) = \sum_m u_m(t) H_m$ such that $U(t)$ satisfies the Schrödinger equation $\dot{U} = -iH(t)U$, with boundary conditions $U(0) = I$ and $U(T) = V$ (we set $\hbar = 1$). Here $\{H_m\}$ is the set of Hamiltonian terms that we can physically implement for the system, and $\{u_m(t)\}$ is a set of real functions that will constitute the control protocol. If we neglect a global phase in V , we can restrict $H(t)$ to the $(n^2 - 1)$ -dimensional space of traceless Hermitian matrices, which we will denote by \mathcal{M} . We divide \mathcal{M} into two subspaces \mathcal{A} and \mathcal{B} , where \mathcal{A} is the subspace of Hamiltonians that we can implement, and \mathcal{B} is the subspace we cannot. We denote a basis for \mathcal{A} by $\{A_j\}$ and a basis for \mathcal{B} by $\{B_k\}$, so that $\{A_j, B_k\}$ is an orthonormal basis for \mathcal{M} . We consider the two physical constraints on H described above: (i) $\|H(t)\| \leq E$, where $\|\cdot\|$ is the Hilbert-Schmidt norm; and (ii) $H(t)$ is restricted to the space \mathcal{A} , so that $H(t) = \sum_j \mu_j(t) A_j$.

Shortest time vs shortest distance.—The following analysis shows why a bound on the norm of the Hamiltonian is a bound on the speed of evolution, meaning that every minimal-time path is a minimal distance path, where distance is defined by the norm. First, because the Hamiltonian appears in the expression $U(t + dt) = e^{-iH(t)dt}U(t)$ multiplied by dt , in any infinitesimal time step, scaling the norm of H by s is equivalent to scaling dt by $1/s$. It follows that for any curve $U(t) = \mathcal{T}(e^{-i \int H(t) dt})$ with $\|H(t)\| \leq E$, \mathcal{T} being the time-ordering operator, the Hamiltonian can be rescaled so that the norm is equal to E at all points on the path, and the path is unchanged but takes a shorter time. This implies that every minimal-time path has $\|H(t)\| = E$. Finally, since the length of every minimal-time path is given by $L = \int_0^T \|H(t)\| dt = \int_0^T E dt = ET$, minimizing the duration T also minimizes the distance L . Thus the minimum-time curve must also be the minimum-distance curve connecting I and V .

Brachistochrone equation.—By virtue of the analysis above, constraint (i) can be replaced by the equality $\text{Tr}[H^2(t)] = E^2$. Because all the constraints are now equalities, we can use the Lagrangian approach to optimization. The resulting Euler-Lagrange equation, often referred to as the QBE, is [28]

$$\dot{H} + \sum_k \dot{\lambda}_k B_k = -i \sum_k \lambda_k [H, B_k], \quad (1)$$

or in terms of the components $\{\mu_j\}$,

$$\dot{\mu}_j = i \sum_l \lambda_l \text{Tr}(H[A_j, B_l]), \quad (2a)$$

$$\dot{\lambda}_k = i \sum_l \lambda_l \text{Tr}(H[B_k, B_l]). \quad (2b)$$

The solution to the QBE involves the two sets of components $\boldsymbol{\mu}(t) = \{\mu_j(t)\}$ and $\boldsymbol{\lambda}(t) = \{\lambda_k(t)\}$, where $H(t) = \sum_j \mu_j(t) A_j$ and $\boldsymbol{\lambda}$ are the Lagrange multipliers, introduced by the constraint (ii). Together with the Schrödinger equation, the QBE [Eq. (1)] defines a boundary value problem for a nonlinear ODE, with the boundary values $U(0) = I$ and $U(T) = V$. Since the minimum-time curve $U(t)$ is uniquely determined by the initial values $\{\mu_j(0), \lambda_k(0)\}$, solving the BVP involves finding the values of $\{\mu_j(0), \lambda_k(0)\}$ and T that give $U(T) = V$. As discussed above, all conventional numerical methods for this BVP convert it into that of solving a set of nonlinear equations. As a result, all these methods suffer a rapidly decreasing performance as the dimension of the ODE increases, failing even for moderately large dimensions.

Geodesic interpretation.—When the control Hamiltonian $H(t)$ is restricted to the subspace \mathcal{A} , the shortest-distance curves that it can generate are no longer the geodesics in the full space of unitaries [38]. Nevertheless, it is possible to derive the geodesic equation for these shortest-distance curves by using a clever trick [35,39]: one introduces a Riemannian metric on \mathcal{M} that applies a penalty to the forbidden subspace \mathcal{B} , so that in the limit when the penalty is large, minimizing the path length also forces $H(t)$ to stay within \mathcal{A} . To do this, we allow the Hamiltonian to be chosen from the entire space \mathcal{M} , so that $H = \sum_j \alpha_j A_j + \sum_k \beta_k B_k$, and define a new inner product, which we will call the “ q inner product,” by

$$\langle H_1, H_2 \rangle_q \equiv \left[\sum_j \alpha_j^{(1)} \alpha_j^{(2)} + q \sum_k \beta_k^{(1)} \beta_k^{(2)} \right]^{1/2}. \quad (3)$$

With this inner product, the metric is $\|H\|_q = \langle H, H \rangle_q$, and the length of a curve $U(t)$ under this q metric is $L = \int \|H(t)\|_q dt$. Since the q metric applies a penalty proportional to q to the basis operators B_k , we can expect that when $q \rightarrow \infty$ the geodesics for the q metric (the “ q geodesics”) will be confined exactly to \mathcal{A} [40]. The q geodesics obey the following geodesic equation, which is the Euler-Lagrange equation for L under the constraint $\|H\|_q = E$ [41]:

$$\mathcal{G}_q(\dot{H}_q) = -i[H_q, \mathcal{G}_q(H_q)], \quad (4)$$

where $\mathcal{G}_q(\cdot) = \mathcal{P}_{\mathcal{A}}(\cdot) + q\mathcal{P}_{\mathcal{B}}(\cdot)$, and $\mathcal{P}_{\mathcal{A}}$ and $\mathcal{P}_{\mathcal{B}}$ project onto the subspaces \mathcal{A} and \mathcal{B} , respectively. In terms of the parameters $\{\alpha_j^{(q)}, \beta_k^{(q)}\}$, the geodesic equation is

$$\begin{aligned}\dot{\alpha}_j^{(q)} &= \text{Tr} \left[iH_q \left(\sum_n \alpha_n^{(q)} [A_j, A_n] + \sum_l q\beta_l^{(q)} [A_j, B_l] \right) \right], \\ \dot{\beta}_k^{(q)} &= \text{Tr} \left[iH_q \left(\sum_n \frac{\alpha_n^{(q)}}{q} [B_k, A_n] + \sum_l \beta_l^{(q)} [B_k, B_l] \right) \right].\end{aligned}\quad (5)$$

We have added the sub- and superscript q to remind us that the control protocol $H(t)$ depends on q .

It is now straightforward to show that when $q \rightarrow \infty$ the geodesic equation becomes the brachistochrone equation, under the assumption that the values $q\beta_k^{(q)}$ remain finite in this limit. First, we note that each of the geodesic equations for the parameters has two terms on the right-hand side, and the second of these constitutes precisely the brachistochrone equation under the replacement $\alpha_j^{(q)} \leftrightarrow \mu_j$ and $q\beta_k^{(q)} \leftrightarrow \lambda_k$. By substituting H into the first term in each of the geodesic equations, we find that the contribution from the components in \mathcal{A} vanishes identically, and that from the components in \mathcal{B} tends to zero as $q \rightarrow \infty$. Minimum-time quantum control protocols can therefore be obtained as the limit of a continuum of geodesics, which makes time-optimal control amenable to the use of geometric tools. This also gives a geometric meaning to the Lagrange multipliers $\{\lambda_k\}$: as H_q is increasingly restricted to \mathcal{A} , and the parameters $\beta_k^{(q)}$ vanish, when scaled by q these values remain finite and become the Lagrange multipliers.

Solving the brachistochrone equation.—Together with the Schrödinger equation, the solution to the geodesic equation is completely determined by specifying the initial value of the Hamiltonian $H_q(0)$. As in the case of the QBE, we do not know what choice for $H_q(0)$ will satisfy the boundary conditions $U(0) = I$ and $U(T) = V$, and thus solve the control problem. However, the geodesic equation has three properties that the brachistochrone does not, and that we can exploit to find fast methods of solving it. These properties are as follows. (i) Since there is a continuum of geodesics, the solution for $q = 1$ can be transformed continuously into the solution for $q = \infty$. This will allow us to obtain $H_q(t)$ for $q \gg 1$ from $H_1(t)$. (ii) For $q = 1$, the solution is trivial: the geodesic equation is merely $\dot{H}_1 = 0$, so the minimal-time control Hamiltonian is constant. Thus $V = \exp(-iH_1T)$ and $H_1 = i \log(V)/T$. Since the logarithm is multiple-valued (has multiple branches), this formula gives a countably infinite set of solutions for H_1 . Further, the choice of T merely scales the norm of H_1 . Thus, it is convenient to set $T = 1$, and the minimum-length protocol is given by the solution for H_1 with the smallest norm (usually the first branch). We expect that it is the minimal-length geodesic that will transform into the minimal-time brachistochrone, although this is not guaranteed. (iii) Any geodesic curve will be uniquely determined by the initial value of $H_q(0)$, unlike the brachistochrone, which requires both $H(0)$ and $\lambda(0)$.

We can now present two simple, fast methods for solving the QBE. The first involves using the fact that there is a continuum of geodesic solutions, parametrized by q , to obtain protocols for $q \gg 1$ from the trivial solutions for $q = 1$. This can be done by deriving an equation for the derivative of $H_q(0)$ with respect to q , and then integrating this equation starting at $q = 1$, a method known as “geodesic deformation” [36]. This procedure is slow, however, and a much faster one, that we will refer to as “ q jumping,” is as follows. We exploit the fact that a geodesic for one value of q is sufficiently close to that for $q + \Delta q$, for some Δq , that we can use it to seed the simple shooting method to quickly obtain the solution for $q + \Delta q$ from that for q . Starting with $q = 1$, and a choice for Δq , we use the shooting method n times to obtain $H_{1+n\Delta q}(0)$ from H_1 . When $n\Delta q$ is large enough, we can use $H_{1+n\Delta q}$ to seed the shooting method to obtain the brachistochrone. There are two caveats to this method. The first is that not all solutions for $q = 1$ continuously deform into solutions for $q = \infty$; a given geodesic can abruptly disappear above some value of q . Thus, we may have to try more than one branch of the logarithm [more than one of the solutions $H_1(t)$] to find the brachistochrone. In this case, we start with the branch for which H_1 has the smallest norm, proceed to the next smallest, and so on. The second caveat is that, if H_1 satisfies $[\mathcal{P}_{\mathcal{A}}(H_1), \mathcal{P}_{\mathcal{B}}(H_1)] = 0$, we cannot start with $q = 1$ (see the Supplemental Material [42]). Fortunately, the shooting method is able to obtain $H_q(0)$ for a low value of q (e.g., $q = 5$) when seeded with a random guess, and having obtained that we proceed as before.

Our second method, which we will call “geodesic search,” is as follows. Due to property (iii) above, any geodesic curve can be found efficiently if we can obtain a good approximation to $H_q(0)$. This can be done by optimizing a weighted sum of two quantities. The first is a measure of the error of the protocol which we quantify using $d = 1 - \|\text{Tr}[V^\dagger U(T)]\|/N$, with N being the dimension of the system. The second quantity is the length of the path under the q norm. The optimal solution for this weighted sum gives a close-to-minimal path that approximately generates V at time T . It is thus a good approximation to $H_q(0)$, from which we can obtain $H_q(0)$ exactly via the simple shooting method, and subsequently the brachistochrone solution, if q is chosen to be sufficiently large. We cannot apply this method to the brachistochrone directly, because there is no way to obtain a good approximation to $\lambda(0)$: the geodesic formulation is essential.

Control in the presence of a drift Hamiltonian.—The methods we have described above can also be used when there is an additional drift Hamiltonian H_0 that cannot be altered by the controller, and which is contained in \mathcal{A} ($H_0 = \sum_j \nu_j A_j$). The total Hamiltonian is $H_{\text{tot}}(t) = H_0 + H(t) \in \mathcal{A}$, and it is the control Hamiltonian that is bounded: $\|H(t)\| \leq E$. In this case, it can be shown

that the time-minimal path still satisfies $\|H(t)\| = E$. The brachistochrone solution can then be analogously derived for this case, and a similar brachistochrone-geodesic connection established. When $H_0 \notin \mathcal{A}$, the situation is more subtle, and will be discussed in a future work.

Example 1: an arbitrary two-qubit evolution.—We consider two qubits whose physical interaction is given by the model

$$H = \hbar \sum_{l,m} \omega_m^{(l)} \sigma_m^{(l)} + \hbar \kappa \sum_m \sigma_m^{(1)} \otimes \sigma_m^{(2)}, \quad (6)$$

where $\sigma_m^{(l)}$, $m = x, y, z$, $l = 1, 2$ are the Pauli operators for the l th qubit. We assume that the experimenter has the ability to vary the six parameters $\{\omega_m^{(l)}\}$ and the interqubit coupling rate κ . The accessible and forbidden spaces for this model are thus $\mathcal{A} = \text{span}\{\sigma_m^{(l)}, \sigma_m^{(1)} \otimes \sigma_m^{(2)}\}$ and $\mathcal{B} = \mathcal{M}/\mathcal{A}$, respectively.

We choose the target unitary V to be a randomly selected two-qubit operator in $\text{SU}(4)$ (the V we use is given in the Supplemental Material [42]). All numerics are run on a 2.6 GHz Intel Core i5. We first attempt to use conventional methods to solve the boundary-value QBE. Running the simple shooting method 100 times with randomly chosen initial guesses fails to obtain a solution, and the multiple-shooting and finite-difference methods have similar behavior. All have great difficulty finding solutions from random initial guesses. We then apply the new methods presented above. Calculating $H_1(0) = i \log(V)$ gives a sequence of solutions which we label with the branch number of the logarithm, $m = 1, 2, \dots$. The norms of these solutions for $H_1(0)$, and thus the corresponding protocol times, increase monotonically with m . Starting with $m = 1$, we attempt to use q jumping to obtain $H_{100}(t)$ from H_1 using steps of size $\Delta q = 1$. This fails for both $m = 1$ and $m = 2$, indicating that these geodesics cannot be extended to $q = 100$. The solution for $m = 3$ succeeds, and takes 32 min. We then use this geodesic to seed the shooting method to find the brachistochrone, which takes 19 s. Of course, to increase our confidence that this is the global minimal-time solution, we must also check that higher values of m do not produce solutions of the QBE with shorter times. We have checked 10 values of m , including those that do not converge, and each takes approximately 30 min, so the total time to obtain the minimal-time protocol is about 5 h.

Next, we use the geodesic-search method. Discretizing the path into 20 segments, minimizing the sum of the error and the path length to obtain an approximate $H_{100}(t)$ usually takes no more than 20 s from an initial random guess. To increase the chance of finding the global minimal-time solution we run 50 searches, which altogether provides 5 different approximate geodesic solutions with $\|H_{100}\|_q < 7$. This takes about 14 min. Using these approximate solutions to seed the shooting method, we find five distinct geodesics $H_{100}(t)$, each taking about 40 s. The

final step is to obtain the brachistochrone starting from the shortest geodesic, just as we did in the method above, and so takes 19 s. The geodesic-search method therefore takes a total time of about 18 min, and thus beats the q jumping method hands-down. Both methods arrive at the same minimum-time protocol, which has a time of $T = 6.69/E$.

Example 2: a CNOT logic gate.—As our second example, we find a time-optimal implementation of the CNOT gate [43], also for the Hamiltonian in Eq. (6). To do so, we first add a global phase of $\pi/4$ to the standard CNOT, so that $V = e^{i\pi/4} U_{\text{CNOT}}$ is in $\text{SU}(4)$. Discretizing the path into 20 segments as above, the geodesic-search method takes about 15 min [about 14 min for the minimization to find the approximation to $H_{100}(t)$, 16 s for the shooting method to obtain $H_{100}(t)$, and 29 s for the shooting method to obtain the brachistochrone.] Using the q jumping method for $m = 1$ to obtain first $H_5(t)$ and then $H_{100}(t)$, using a step size $\Delta q = 1$, takes a total time of 21.5 min, and finding the brachistochrone from $q = 100$ takes 28 s for a total time of 22 min. In fact, for this problem, we find that $q = 50$ is sufficient to obtain the brachistochrone, reducing the total time to 9 min. We similarly determine the solutions of the QBE that result from the branches $m = 2, \dots, 10$, which takes a total of about 1.5 h. The geodesic-search method is thus faster for this example as well. The minimum protocol time we obtain is $T = 5.75/E$. We plot the seven components $\{\mu_j(t)\}$ of the brachistochrone $H(t)$ in Fig. 1, along with the seven components $\{\alpha_j(t)\}$ of the geodesic solution $H_{100}(t)$ for comparison.

Although q jumping is slower than the geodesic-search method, it has the advantage of enumerating a set of solutions, providing confidence that we have obtained the global time-optimal solution. To maximize the probability of obtaining this global optimum, we suggest applying both methods to compare their solutions.

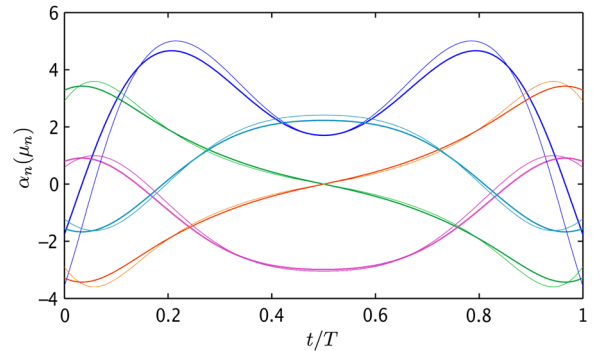


FIG. 1 (color online). Solid lines: the seven control functions $\mu_k(t)$, $k = 1, \dots, 7$, that implement the minimal-time (brachistochrone) CNOT gate for a given two-qubit interaction. Dashed lines: the seven functions $\alpha_k(t)$ for the geodesic protocol with $q = 100$ (see text), which is used to obtain the brachistochrone. Two pairs of control functions are identical, so only five distinct curves appear for both protocols.

Conclusion.—We have revealed a fundamental connection between time-optimal control and geodesics in the space of unitary operators. This connection opens up time-optimal control to the tools of geometry, and as such we expect it to have broad applications within quantum control. One such application we presented here, obtaining a practical method for solving the quantum brachistochrone. We suggest that further applications could include time-optimal control in the presence of arbitrary drift Hamiltonians, and the computational complexity of quantum control under constraints on the available Hamiltonians.

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- [42] See Supplemental Material at <http://link.aps.org/supplemental/10.1103/PhysRevLett.114.170501> for a detailed proof of the brachistochrone-geodesic connection, further details of the two examples in the text, MATLAB code for Example 2, and an extension of our results to the situation in which there is a fixed "drift" Hamiltonian in the space of controls.
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