Shortest evolution path between two mixed states and its realization

Jie-Hui Huang,[1] Shan-Shan Dong,[1] Guang-Long Chen,[1] Nan-Run Zhou,[2] Fu-Yao Liu,[1,*] and Li-Guo Qin[1,†]
[1]*School of Mathematics, Physics, and Statistics, Shanghai University of Engineering Science, Shanghai 201620, China*
[2]*School of Electronic and Electrical Engineering, Shanghai University of Engineering Science, Shanghai 201620, China*

(Received 10 December 2023; accepted 25 March 2024; published 8 April 2024)

In a quantum unitary system, an initial state may have different paths to evolve to a target state, and the only requirement is that the initial and target states share the same eigenvalue spectrum. We focus on the evolution between two nondegenerate mixed states in this paper, and investigate the shortest evolution path between them. By minimizing the path distance contained in the unitary operator connecting the initial and target states over a series of phases, the shortest evolution path could be figured out. This minimum path distance has an analytical form in the single-qubit dynamical system, and its solution in the three- or higher-dimensional dynamical system could be obtained numerically. Based on the unitary operator associated with the shortest evolution path, a general form for the Hamiltonian to realize it is presented. Here we present another way to study quantum optimal control, which is based on the path distance between the initial state and its evolution state, rather than the state distance between them.

DOI: 10.1103/PhysRevA.109.042405

I. INTRODUCTION

The issue of quantum evolution attracts much attention in recent years owing to its important role in quantum information processing, which takes effect on the computational capacity of quantum computation [1,2], transferring rate of information [3–5], measurement precision in quantum metrology [6–8], entropy production rate in nonequilibrium quantum processes [9,10], charging power of quantum batteries [11,12], and so on. How to evolve a quantum state to a target state as fast as possible becomes a hot topic in this field. Several techniques are developed with this aim, such as the Krotov algorithm [13,14], a numerical recursive method based on the Lagrange multiplier problem [15,16], and the variational method based on the quantum brachistochrone problem [17]. Whether there exists a geodesic evolution between two given states is another interesting question. If a pure state $|\psi_0\rangle$ is to evolve to another pure state $|\psi_\tau\rangle$ in a unitary system, a geodesic evolution between them could be realized by imposing the Hamiltonian $H = g|\psi_0\rangle\langle\psi_\tau| + \text{H.c.}$ onto the system, where the coupling strength g determines the time required to accomplish this evolution, and the evolution state is always in the plane spanned by $|\psi_0\rangle$ and $|\psi_\tau\rangle$. However, it seems hard to define the geodesic evolution between two mixed states. Although we have no answer for the geodesic evolution between two mixed states, a related question attracts our attention recently: what is the shortest evolution path between two mixed states?

In a quantum unitary system, an initial mixed state ρ_0 turns to its evolution state ρ_t through the transformation $\rho_t = U_t\rho_0 U_t^\dagger$. Here the unitary operator U_t is determined by the Hamiltonian through the relation $U_t = \mathcal{T}\exp\{-i\int_0^t H(t')dt'\}$, where we set the constant $\hbar = 1$ hereafter, and $\mathcal{T}$ is the time-ordering operator. The unitary operator U_t represents one evolution path from the initial state ρ_0 to the evolution state ρ_t in the following. In Ref. [18], the path distance contained in an Nth-order unitary operator U_t is defined as

$$d(U_t) = \pi - \tfrac{1}{2}\max\{D_j\}, \tag{1a}$$

with

$$D_j = \begin{cases} \phi_{j+1} - \phi_j, & \text{for } j = 1, 2, \ldots, N-1 \\ 2\pi + \phi_1 - \phi_N, & \text{for } j = N. \end{cases} \tag{1b}$$

Here $\{D_j\}$ is the set of phase differences between neighboring eigenvalues of U_t, which are aligned based on their principal argument (phase) in ascending order, $\phi_j \leqslant \phi_{j+1}$. The principal argument of every eigenvalue is confined in the range $(-\pi, \pi]$. The path distance defined in this way is actually the minimum rotation angle of a state vector in the Hilbert space under the action of this unitary operator, which satisfies three requirements for a good measure of distance: positivity, symmetry, and triangle inequality [19,20]. It is proven that the path distance contained in U_t is an upper bound of the Bures distance between any two quantum states connected by U_t, i.e., $d(U_t) \geqslant d_B(\rho_0, \rho_t)$, if $\rho_t = U_t\rho_0 U_t^\dagger$. The Bures distance [21] between two quantum states ρ_0 and ρ_t is defined as the arccosine of the Uhlmann fidelity between them [22,23]:

$$d_B(\rho_0, \rho_t) = \arccos \mathcal{F}(\rho_0, \rho_t), \tag{2a}$$

with

$$\mathcal{F}(\rho_0, \rho_t) = \text{Tr}\Big[\sqrt{\sqrt{\rho_0}\rho_t\sqrt{\rho_0}}\Big]. \tag{2b}$$

If two mixed states share the same eigenvalue spectrum, they could evolve to each other via different evolution paths, and each path contains its own path distance. For example, under the action of the Hamiltonian $H_1 = \left(\begin{smallmatrix} 0 & 0 \\ 0 & 1 \end{smallmatrix}\right)$, a mixed state $\rho_0 = \frac{1}{4}\left(\begin{smallmatrix} 2 & 1 \\ 1 & 2 \end{smallmatrix}\right)$ turns to a target state $\rho_\tau = \frac{1}{4}\left(\begin{smallmatrix} 2 & i \\ -i & 2 \end{smallmatrix}\right)$ at

*liu-fuyao@163.com
†lgqin@foxmail.com

time $t = \pi/2$. The corresponding unitary evolution operator is $U_1 = \exp\{-i\int_0^{\frac{\pi}{2}} H_1 dt\} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & -i \end{smallmatrix}\right)$ with path distance $d(U_1) = \pi/4$. On the other hand, the evolution from ρ_0 to ρ_τ could also be realized through the unitary evolution operator $U_2 = \frac{1}{\sqrt{2}} e^{i(2\sqrt{3}+3)\pi/36} \left(\begin{smallmatrix} e^{i\pi/6} & e^{-i\pi/3} \\ -e^{i\pi/6} & e^{-i\pi/3} \end{smallmatrix}\right)$, which contains path distance $d(U_2) = \pi/3$. The unitary operator U_2 describes the action of the Hamiltonian $H_2 = \frac{1}{\sqrt{11}} \left(\begin{smallmatrix} -3/2 & 1+i \\ 1-i & 1/2 \end{smallmatrix}\right)$ with the interaction time $t = \sqrt{33}/9$, i.e., $U_2 = \exp\{-i\int_0^{\sqrt{33}/9} H_2 dt\}$. The path distance contained in U_1 is different from that in U_2, which are both larger than the Bures distance between the two states ρ_0 and ρ_τ with $d_B(\rho_0, \rho_\tau) = \arccos(\sqrt{14}/4)$.

Quantum evolution would result in the change of the distance between the initial state and its evolution state, and the path distance could then be regarded as one property of the evolution itself. If we replace state distance by path distance in some issues, different conclusions might be made. For example, if we define the evolution speed of a quantum system as the changing rate of the path distance, rather than the changing rate of the state distance, then the instantaneous evolution speed depends on the Hamiltonian only [24].

In this paper, we present the general form of the unitary operator for connecting two given mixed states, and minimize the path distance contained in the general unitary operator to figure out the shortest evolution path. The analytical solution for the minimum path distance could be obtained in a single-qubit system. We also use a single-qutrit example to illustrate how to minimize the path distance in a higher-dimensional system numerically. Based on the unitary operator associated with the shortest evolution path, we present the Hamiltonian to realize it finally.

II. SHORTEST EVOLUTION PATH

A. General form of the unitary operator for the evolution between two mixed states

We start the analysis on the shortest evolution path between two mixed states with the eigenvalue decomposition of a mixed state, $\rho_0 = V_0 \Lambda V_0^\dagger$. Here Λ is a diagonal matrix composed of the eigenvalues of ρ_0, $\Lambda_{kk} = \lambda_k$. For simplicity, we only consider the nondegenerate mixed state, and assume that the eigenvalues $\{\lambda_k\}$ are arranged in ascending order, $\lambda_k < \lambda_{k+1}$. The eigenvectors of ρ_0 compose the matrix V_0 with $V_0 = (|\psi_1\rangle \ |\psi_2\rangle \cdots |\psi_N\rangle)$, where the kth eigenvector $|\psi_k\rangle$ is associated with the kth eigenvalue λ_k. In fact, the matrix V_0 is not unique for a mixed state, because the overall phase of each eigenvector could not be confirmed from ρ_0. So we rewrite the eigenvalue decomposition of ρ_0 as

$$\rho_0 = V_0 M_\varphi \Lambda M_\varphi^\dagger V_0^\dagger, \tag{3}$$

where the diagonal matrix M_φ is composed of the overall phase $\{\varphi_k\}$ of the eigenvectors of ρ_0:

$$M_\varphi = \begin{pmatrix} e^{i\varphi_1} & 0 & 0 & 0 \\ 0 & e^{i\varphi_2} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & e^{i\varphi_N} \end{pmatrix}. \tag{4}$$

Since the matrix M_φ is a unitary matrix, we call it the phase operator hereafter. In fact, the equality $M_\varphi \Lambda M_\varphi^\dagger = \Lambda$ holds for arbitrary M_φ, no matter what values the overall phases $\{\varphi_k\}$ are.

Since the eigenvalues of a mixed state keep invariant during a unitary evolution, the evolution state ρ_t has the following eigenvalue decomposition:

$$\rho_t = V_t M_{\varphi'} \Lambda M_{\varphi'}^\dagger V_t^\dagger, \tag{5}$$

where V_t is composed of the eigenvectors of ρ_t, $V_t = (|\psi_1'\rangle \ |\psi_2'\rangle \cdots |\psi_N'\rangle)$. The phase operator $M_{\varphi'}$ has a similar form as M_φ in Eq. (4), which contains the overall phase of the eigenvectors $\{|\psi_k'\rangle\}$. At the same time, the evolution state ρ_t could also be described through the unitary evolution operator U_t and the initial state ρ_0 as $\rho_t = U_t \rho_0 U_t^\dagger$. By substituting the two forms (3) and (5) into this equation, we derive the general form of the unitary operator U_t for the evolution from ρ_0 to ρ_t:

$$U_t = V_t M_{\varphi'} M_\varphi^\dagger V_0^\dagger = V_t M_{\varphi''} V_0^\dagger, \tag{6}$$

where $M_{\varphi''} = M_{\varphi'} M_\varphi^\dagger$ is also a phase operator in the form (4).

B. Shortest evolution path and the corresponding time-independent Hamiltonian

Now we consider the evolution from the initial state $\rho_0 = V_0 \Lambda V_0^\dagger$ to a target state $\rho_\tau = V_\tau \Lambda V_\tau^\dagger$. By substituting the unitary operator $U_\tau = V_\tau M_\varphi V_0^\dagger$ in Eq. (6) into the path distance in Eq. (1) and optimizing it over the set of the phase operators $\{M_\varphi\}$, we obtain the minimum path distance of the unitary evolution from ρ_0 to ρ_τ:

$$d_P(\rho_0, \rho_\tau) = \min_{\{M_\varphi\}} d(V_\tau M_\varphi V_0^\dagger). \tag{7}$$

As we mentioned above, V_0 and V_τ are composed of the eigenvectors of the mixed states ρ_0 and ρ_τ, respectively. The kth eigenvectors of V_0 and V_τ, $|\psi_k\rangle$ and $|\psi_k'\rangle$, are associated with the same eigenvalue λ_k. The phases $\{\phi_k\}$ in the operator M_φ are variable. Because the path distance contained in a unitary operator is determined by the eigenvalues of the operator, and the matrix $V_\tau M_\varphi V_0^\dagger$ has the same eigenvalue spectrum as the matrix $V_0^\dagger V_\tau M_\varphi$, the minimum path distance of the evolution from ρ_0 to ρ_τ could also be written as

$$d_P(\rho_0, \rho_\tau) = \min_{\{M_\varphi\}} d(V_0^\dagger V_\tau M_\varphi). \tag{8}$$

Once the unitary operator associated with the shortest evolution path is ready, the Hamiltonian $H(t)$ to realize it should satisfy $U_\tau = \mathcal{T} \exp\{-i\int_0^\tau H(t)dt\}$. For the sake of simplicity, we only consider the time-independent Hamiltonian here, and this relation is simplified as $U_\tau = \exp(-iH\tau)$. The Hamiltonian could then be figured out:

$$H = \frac{i}{\tau} \ln U_\tau + R. \tag{9}$$

Here the real parameter τ could be used to control the energy spread of the system, which is also the interaction time required to realize the unitary operator U_τ. The real number R, which only induces an overall phase to the evolution state, could be used to control the average energy of the system. The above equation (9) presents a general solution of the time-

independent Hamiltonian for realizing the unitary operator U_τ, no matter what values τ and R are.

III. SHORTEST EVOLUTION PATH BETWEEN TWO SINGLE-QUBIT STATES

In this section, we use a single-qubit example to illustrate the optimization of path distance. Here we aim at an analytical solution of minimizing the path distance contained in a general second-order evolution operator, which could be derived by driving a fix state to a parametrized state. Since any mixed state has a diagonal form in the basis composed of its own eigenvectors, we assume the initial state of this single-qubit system has a diagonal form for simplicity:

$$\rho_0 = \frac{1}{4}\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}. \tag{10}$$

According to Eq. (6), a general evolution operator between two mixed states is determined by their eigenvectors, combined with a phase operator, and the eigenvalues play no role in the quantification of path distance. In a quantum unitary system, the target state should have the same spectrum as the initial one, so we assume the parametrized target state has the following form:

$$\rho_\tau = \frac{1}{4}\begin{pmatrix} 1+2\sin^2\theta & -\sin 2\theta e^{i\alpha} \\ -\sin 2\theta e^{-i\alpha} & 1+2\cos^2\theta \end{pmatrix}, \quad \left[\theta \in \left(0, \frac{\pi}{2}\right)\right]. \tag{11}$$

The decomposition of the two mixed states is $\rho_0 = V_0 \Lambda V_0^\dagger$ and $\rho_\tau = V_\tau \Lambda V_\tau^\dagger$ with $\Lambda = \rho_0$. V_0 and V_τ are composed of the eigenvectors of ρ_0 and ρ_τ, respectively. In fact, V_0 is the second-order identity matrix, and

$$V_\tau = \begin{pmatrix} \cos\theta & \sin\theta e^{i\alpha} \\ \sin\theta e^{-i\alpha} & -\cos\theta \end{pmatrix}. \tag{12}$$

According to Eq. (6), the general form of the unitary operator U_τ describing the evolution from ρ_0 to ρ_τ is $U_\tau = V_\tau M_\varphi V_0^\dagger$, with M_φ being the phase operator in the form (4), so we have

$$U_\tau = \begin{pmatrix} \cos\theta e^{i\varphi_1} & \sin\theta e^{i(\varphi_2+\alpha)} \\ \sin\theta e^{i(\varphi_1-\alpha)} & -\cos\theta e^{i\varphi_2} \end{pmatrix}. \tag{13}$$

Please note that this is a general form of the second-order unitary operator, which has four variable parameters: θ, α, φ_1, and φ_2.

In order to obtain the analytical result of the path distance contained in U_τ, we need write out its eigenvalues, $\lambda_1 = e^{i\phi_1}$ and $\lambda_2 = e^{i\phi_2}$, with the arguments $\phi_1 = \frac{\varphi_1+\varphi_2}{2} + \arcsin[\cos\theta \sin(\frac{\varphi_1-\varphi_2}{2})]$ and $\phi_2 = \frac{\varphi_1+\varphi_2}{2} + \pi - \arcsin[\cos\theta \sin(\frac{\varphi_1-\varphi_2}{2})]$. Based on the definition in Eq. (1), the path distance of the unitary operator U_τ is

$$\begin{aligned} d(U_\tau) &= \frac{\pi}{2} - \arcsin\left|\cos\theta \sin\left(\frac{\varphi_1-\varphi_2}{2}\right)\right| \\ &= \arccos\left|\cos\theta \sin\left(\frac{\varphi_1-\varphi_2}{2}\right)\right|. \end{aligned} \tag{14}$$

By substituting this result into the minimum path distance in Eq. (7) and optimizing it over the two phases φ_1 and φ_2, we obtain the minimum path distance of the evolution from ρ_0 to ρ_τ:

$$\begin{aligned} d_P(\rho_0, \rho_\tau) &= \min_{\{M_\varphi\}} d(U_\tau) \\ &= \min_{\{\varphi_1,\varphi_2\}} \arccos\left|\cos\theta \sin\left(\frac{\varphi_1-\varphi_2}{2}\right)\right|. \end{aligned} \tag{15}$$

The path distance reaches its minimum value $d_P(\rho_0, \rho_\tau) = \theta$ when $\sin(\frac{\varphi_1-\varphi_2}{2}) = 1$. If we set $\varphi_1 = 0$ and $\varphi_2 = -\pi$ for simplicity, the unitary operator U_τ is

$$U_\tau = V_\tau M_\varphi V_0^\dagger = \begin{pmatrix} \cos\theta & -\sin\theta e^{i\alpha} \\ \sin\theta e^{-i\alpha} & \cos\theta \end{pmatrix}. \tag{16}$$

This unitary operator U_τ describes the shortest evolution path from ρ_0 and ρ_τ, and the minimum path distance is $d_P(\rho_0, \rho_\tau) = \theta$.

IV. OPTIMAL CONTROL BETWEEN TWO MIXED SINGLE-QUTRIT STATES

The minimization of path distance contained in a unitary operator is made over a phase matrix in Eq. (4). In an N-dimensional quantum system, this matrix contains N independent phases. Since an overall phase plays no role in the measurement of a physical quantity, we can fix one phase and consider the rest $(N-1)$ independent phases in the optimization. So only one variable needs to be considered in the optimization of path distance in a single-qubit system, which could be solved analytically. However, the situation becomes complicated when the dimensionality of the system increases, where more variables have to be considered in the optimization and the eigenvalues of a general third- or higher-order unitary operator could hardly be solved analytically. In a word, the minimum evolution path in a three- or higher-dimensional system needs be solved numerically, and $(N-1)$ variables are to be considered in the optimization of path distance in an N-dimensional system.

In this section, we investigate the shortest evolution of a single-qutrit state numerically. Two rules are obeyed for the choice of the initial and target states.

(i) The initial and target states have to be described by two nondegenerate full-rank matrices to avoid trivial results.

(2) An analytical Hamiltonian could be used to drive the initial state to the target state.

Just as done in the above single-qubit example, we study the evolution of a mixed single-qutrit state ρ_0 in the basis composed of its own eigenvectors, and assume it has the following diagonal form:

$$\rho_0 = \frac{1}{6}\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix}, \tag{17}$$

where the eigenvalues in the diagonal elements play no role in the quantification of path distance. The target state is set as follows:

$$\rho_\tau = \frac{1}{36}\begin{pmatrix} 13 & 4+i & 2-2i \\ 4-i & 13 & 2+2i \\ 2+2i & 2-2i & 10 \end{pmatrix}. \tag{18}$$

This target state could be achieved by imposing the Hamiltonian,

$$H_1 = \begin{pmatrix} 1 & 7 & -4 \\ 7 & 1 & -4 \\ -4 & -4 & 4 \end{pmatrix}, \tag{19}$$

onto the system with the interaction time $\tau = \pi/12$, the matrix elements of which are all integers. The evolution under this action could be described by the following unitary operator:

$$U_\tau = \exp\{-i\int_0^{\frac{\pi}{12}} H_1 dt\} = \frac{1}{6}\begin{pmatrix} -1+3i & -1-3i & 4 \\ -1-3i & -1+3i & 4 \\ 4 & 4 & 2 \end{pmatrix}, \tag{20}$$

which satisfies $\rho_\tau = U_\tau \rho_0 U_\tau^\dagger$.

The three eigenvalues of the above U_τ are $\lambda_1 = 1$, $\lambda_2 = i$, and $\lambda_3 = -1$, with principal arguments $\phi_1 = 0$, $\phi_2 = \pi/2$, and $\phi_3 = \pi$, respectively. Based on the definition in Eq. (1), the path distance contained in U_τ is $d(U_\tau) = \pi/2$, which is larger than the Bures distance between ρ_0 and ρ_τ with $d_B(\rho_0, \rho_\tau) \approx 0.3313$.

We want to know whether the evolution path represented by the above unitary operator (20) is the shortest one among all potential evolution paths from the initial state (17) to the target state (18), and how to find out the shortest evolution if the answer is "no."Following the steps introduced in Eqs. (6)–(8), we first write out the eigenvalue decomposition of the initial and target states as $\rho_0 = V_0 \Lambda V_0^\dagger$ and $\rho_\tau = U_\tau \Lambda U_\tau^\dagger$ with $\Lambda = \rho_0$ and V_0 being the third-order identity matrix here. According to Eq. (6), a general form for describing the evolution from ρ_0 to ρ_τ is

$$U_{\{\varphi\}} = U_\tau M_\varphi V_0^\dagger = \frac{1}{6}\begin{pmatrix} \sqrt{10}e^{i(\varphi_1+\theta_0)} & \sqrt{10}e^{i(\varphi_2-\theta_0)} & 4e^{i\varphi_3} \\ \sqrt{10}e^{i(\varphi_1-\theta_0)} & \sqrt{10}e^{i(\varphi_2+\theta_0)} & 4e^{i\varphi_3} \\ 4e^{i\varphi_1} & 4e^{i\varphi_2} & 2e^{i\varphi_3} \end{pmatrix}, \tag{21}$$

where θ_0 is the argument of the complex number $\theta_0 = \arg(-1+3i)$. Then the shortest evolution path between ρ_0 and ρ_τ could be obtained by minimizing its path distance over all involved phases:

$$d_P(\rho_0, \rho_\tau) = \min_{\{\varphi_1,\varphi_2,\varphi_3\}} d[U_{\{\varphi\}}]. \tag{22}$$

Since an overall phase of a unitary operator plays no role in the quantification of the path distance contained in it, the optimization of the above path distance (22) could be simplified as

$$d_P(\rho_0, \rho_\tau) = \min_{\{\delta\phi_1,\delta\phi_2\}} d[U_{\{\delta\phi\}}], \tag{23}$$

with

$$U_{\{\delta\phi\}} = e^{-i\varphi_3} U_{\{\varphi\}} = \frac{1}{6}\begin{pmatrix} \sqrt{10}e^{i(\delta\phi_1+\theta_0)} & \sqrt{10}e^{i(\delta\phi_2-\theta_0)} & 4 \\ \sqrt{10}e^{i(\delta\phi_1-\theta_0)} & \sqrt{10}e^{i(\delta\phi_2+\theta_0)} & 4 \\ 4e^{i\delta\phi_1} & 4e^{i\delta\phi_2} & 2 \end{pmatrix}. \tag{24}$$

Here only two variables $\delta\phi_1 \equiv \varphi_1 - \varphi_3$ and $\delta\phi_2 \equiv \varphi_2 - \varphi_3$ are involved in the minimization, which is equivalent to the minimization of the path distance contained in $U_{\{\varphi\}}$ in Eq. (21) by fixing one phase, $\varphi_3 = 0$. The two phase differences $\delta\phi_1$ and $\delta\phi_2$ are both confined in the range $(-\pi, \pi]$, so the numerical result of the minimum path distance, based on the definition (1), could be obtained through the steepest descent method or Newton's method.

In Fig. 1, we plot the path distance contained in the unitary operator (24) as a function of the two variables $\delta\phi_1$ and $\delta\phi_2$. Each point in the curved surface has a projection point in the $\delta\phi_1$-$\delta\phi_2$ plane, and thus corresponds to a unitary operator $U_{\{\delta\phi\}}$ in Eq. (24), which turns the initial state ρ_0 to the target state ρ_τ. The function value of each point in the curved surface means the path distance contained in the corresponding unitary operator. The path distance of the unitary operator (24) is evaluated in the range about [1.2490, 2.0944], and the precision of our numerical results is of the order of 10^{-7}. In principle, the path distance of an Nth-order unitary operator is no larger than $(N-1)\pi/N$ [18], so the value range of the path distance contained in a third-order unitary operator is $[0, 2\pi/3]$. It is shown that the path distance of the evolution between ρ_0 and ρ_τ is larger than the Bures distance between ρ_0 and ρ_τ with $d_B(\rho_0, \rho_\tau) \approx 0.3313$, no matter which evolution path is chosen.

Since the minimum path distance contained in the above unitary operator $U_{\{\delta\phi\}}$ (24) is about 1.2490 over all allowed $\delta\phi_1$ and $\delta\phi_2$, then the minimum path distance between ρ_0 and ρ_τ is 1.2490 according to its definition in Eq. (7), i.e., $d_P(\rho_0, \rho_\tau) \simeq 1.2490$. This minimum path distance corresponds to the phase difference $\delta\phi_1 = \delta\phi_2 \simeq -2.4981$ in our numerical results. The shortest evolution path between ρ_0 and ρ_τ is then described by the following unitary operator:

$$U_s \simeq \begin{pmatrix} 0.4333 - 0.3i & -0.1667 + 0.5i & 0.6667 \\ -0.1667 + 0.5i & 0.4333 - 0.3i & 0.6667 \\ -0.5333 - 0.4i & -0.5333 - 0.4i & 0.3333 \end{pmatrix}. \tag{25}$$

The following question is how to realize the above unitary operator U_s for the shortest evolution. By substituting this unitary operator into the Hamiltonian in Eq. (9), we obtain the Hamiltonian corresponding to this shortest evolution path:

$$H \simeq \frac{1}{\tau}\begin{pmatrix} 0.2334 & -0.6939 & 0.2776 + 0.8327i \\ -0.6939 & 0.2334 & 0.2776 + 0.8327i \\ 0.2776 - 0.8327i & 0.2776 - 0.8327i & -0.1830 \end{pmatrix} + R. \tag{26}$$

Here the parameter τ indicates the evolution time required to realize the unitary operator U_s in Eq. (25) under the action of the above Hamiltonian, which could be used to control the energy variance of the system. The constant R in the Hamiltonian, which induces an overall phase to the evolution state, could be used to control the average energy. Although

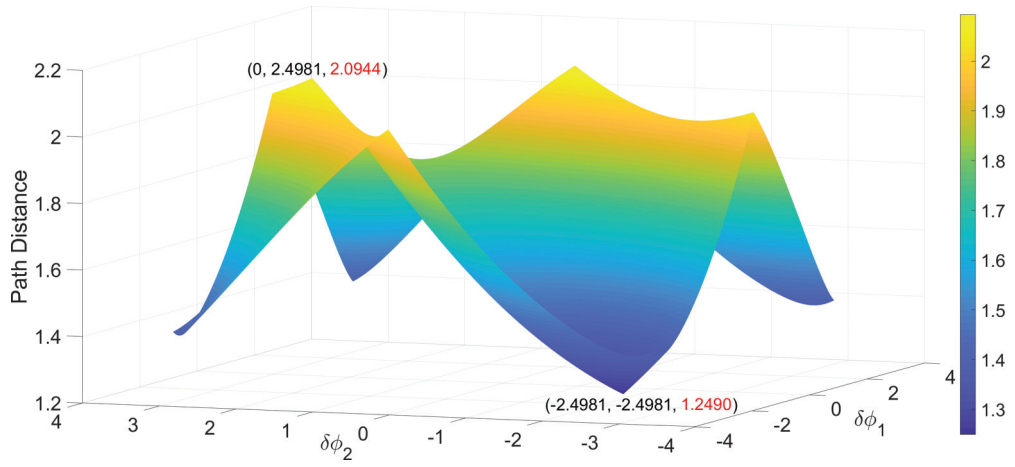

FIG. 1. Numerical results of the path distance contained in the unitary operator (24) as a function of the two parameters $\delta\phi_1$ and $\delta\phi_2$. The maximum path distance $d(U_{\{\delta\phi\}}) \simeq 2.0944$ occurs at $\delta\phi_1 = 0$ and $\delta\phi_2 \simeq 2.4981$, and the minimum path distance $d(U_{\{\delta\phi\}}) \simeq 1.2490$ occurs at $\delta\phi_1 = \delta\phi_2 \simeq -2.4981$. Each point in the curved surface corresponds to a unitary operator turning the initial state ρ_0 (17) to the target state ρ_τ (18), thus describes an evolution path from ρ_0 to ρ_τ. Although these paths connect the same pair of states, they may contain different path distances.

different values of τ and R in the above Hamiltonian would result in different evolution speeds of the system, as well as different overall phases to the evolution state, they in fact correspond to the same evolution path, because every Hamiltonian in Eq. (26) governs the system from ρ_0 (17) to ρ_τ (18) along the shortest evolution path, no matter what values τ and R are.

Particularly, if we set the evolution time as $\tau = 0.1684$ and the constant $R = 2.3503$, then the above Hamiltonian has an explicit form:

$$H_2 = \begin{pmatrix} 3.7360 & -4.1199 & 1.6479 + 4.9439i \\ -4.1199 & 3.7360 & 1.6479 + 4.9439i \\ 1.6479 - 4.9439i & 1.6479 - 4.9439i & 1.2640 \end{pmatrix}. \tag{27}$$

It is found that the expectation value and variance of this Hamiltonian H_2, imposed onto the initial state ρ_0, are equal to the expectation value and variance of the above Hamiltonian H_1 in Eq. (19) imposed on the same state, i.e., $\bar{E}_1 = \bar{E}_2 = 2.5$ and $\Delta^2 E_1 = \Delta^2 E_2 = 50.75$ with $\bar{E}_i = \langle H_i \rangle$ and $\Delta^2 E_i = \langle H_i^2 \rangle - \bar{E}_i^2$ $(i = 1, 2)$. Please note that the average energy and its variance remain unchanged during a unitary evolution in a time-independent quantum system. Here we see that the two forms of Hamiltonian, H_1 in Eq. (19) and H_2 in Eq. (27), both drive the initial state ρ_0 (17) to the target state ρ_τ (18), with the same average energy and energy variance, but the time required for accomplishing the evolution is difference. The required evolution time for H_1 is $\tau_1 = \pi/12$, which is longer than the evolution time $\tau_2 = 0.1684$ for H_2. That is to say, the average energy and the energy spread of a quantum system are not the only factors to determine the evolution speed of the system, and maybe other moments of the energy spectra should be taken into account [25].

V. CONCLUSIONS

To summarize, the evolution path connecting two given mixed states is not unique, and a general unitary operator for describing such an evolution could be represented by the production of three matrices including unitary operators composed of the eigenvectors of the initial and target states and a diagonal phase operator. The path distance contained in a unitary operator could be considered as the minimum rotation angle imposed on a quantum state. The path distance defined in this way depends on the unitary operator itself, and is independent of the state. As a matter of fact, the length of a path connecting two points is no smaller than the distance between the two points in the classical kinematics. Its quantum analog is also valid, i.e., the path distance contained in a unitary operator in a quantum dynamics is no smaller than the state distance between any pair of states connected through this unitary operator. The shortest evolution path between two mixed states could be derived through the optimization of the path distance over $(N-1)$ independent phases in an N-dimensional system, the solution of which could be obtained in a single-qubit system analytically, or in a single-qutrit system numerically. Once the unitary operator associated with the shortest evolution path is figured out, the general form of the time-independent Hamiltonian for realizing it is presented with two controllable parameters. Different from the usual way by minimizing the evolution time, here we provide another way to study quantum optimal control based on the path distance.

Besides quantum optimal control, path distance has some other potential applications in quantum information

processing. For example, the path distance of a unitary operator is an upper bound of the distance between two quantum states connected through it, which could be used for estimating the fidelity between two unknown states, given the evolution operator between them. Furthermore, the evolution speed of a quantum system, usually defined as the changing rate of the distance between the initial state and its evolution state, has a limit so that the evolution time from the initial state to the target state has a lower bound [26–30] and the quantum speed limit is extended in open systems [31,32], thermal states [33], and others cases [34–37]. The quantum speed limit is usually ascribed to the energy spectra of the quantum system. However, if we define the evolution speed as the changing rate of path distance, rather than the state distance, then the quantum speed limit could be interpreted in another way, which is determined by the Hamiltonian, rather than the energy spectra of the system, because the path distance is determined by the evolution operator only and independent of the quantum state. Since the path distance is in fact a map from the set of unitary operators to the set of non-negative numbers, it could be used potentially in the issues where certain magnitude information contained in a unitary operator is under consideration. For example, *quantum complexity* provides an operational definition for quantifying the "cost" of simulating a unitary operator [38–41], which is widely used in several topics such as distinguishing chaotic systems from integrable ones [42], studying black holes [43], and quantifying state complexity in continuous many-body quantum systems [44].

ACKNOWLEDGMENTS

This work was supported by National Natural Science Foundation of China (NSFC) Projects No. 11664018, No. 12174247, and No. U2031145.

[1] S. Lloyd, Ultimate physical limits to computation, Nature (London) **406**, 1047 (2000).
[2] S. Lloyd, Computational capacity of the universe, Phys. Rev. Lett. **88**, 237901 (2002).
[3] J. D. Bekenstein, Energy cost of information transfer, Phys. Rev. Lett. **46**, 623 (1981).
[4] M. Murphy, S. Montangero, V. Giovannetti, and T. Calarco, Communication at the quantum speed limit along a spin chain, Phys. Rev. A **82**, 022318 (2010).
[5] B. Mohan, S. Das, and A. K. Pati, Quantum speed limits for information and coherence, New J. Phys. **24**, 065003 (2022).
[6] V. Giovannetti, S. Lloyd, and L. Maccone, Quantum metrology, Phys. Rev. Lett. **96**, 010401 (2006).
[7] V. Giovannetti, S. Lloyd, and L. Maccone, Advances in quantum metrology, Nat. Photonics **5**, 222 (2011).
[8] A. W. Chin, S. F. Huelga, and M. B. Plenio, Quantum metrology in non-Markovian environments, Phys. Rev. Lett. **109**, 233601 (2012).
[9] S. Deffner and E. Lutz, Generalized Clausius inequality for nonequilibrium quantum processes, Phys. Rev. Lett. **105**, 170402 (2010).
[10] A. del Campo, J. Goold, and M. Paternostro, More bang for your buck: Super-adiabatic quantum engines, Sci. Rep. **4**, 6208 (2014).
[11] F. C. Binder, S. Vinjanampathy, K. Modi, and J. Goold, Quantacell: Powerful charging of quantum batteries, New J. Phys. **17**, 075015 (2015).
[12] F. Campaioli, F. A. Pollock, F. C. Binder, L. Céleri, J. Goold, S. Vinjanampathy, and K. Modi, Enhancing the charging power of quantum batteries, Phys. Rev. Lett. **118**, 150601 (2017).
[13] V. F. Krotov, *Global Methods in Optimal Control Theory* (Marcel Dekker, New York, 1996).
[14] T. Caneva, M. Murphy, T. Calarco, R. Fazio, S. Montangero, V. Giovannetti, and G. E. Santoro, Optimal control at the quantum speed limit, Phys. Rev. Lett. **103**, 240501 (2009).
[15] A. P. Peirce, M. A. Dahleh, and H. Rabitz, Optimal control of quantum-mechanical systems: Existence, numerical approximation, and applications, Phys. Rev. A **37**, 4950 (1988).
[16] T. Calarco, U. Dorner, P. S. Julienne, C. J. Williams, and P. Zoller, Quantum computations with atoms in optical lattices: Marker qubits and molecular interactions, Phys. Rev. A **70**, 012306 (2004).
[17] A. Carlini, A. Hosoya, T. Koike, and Y. Okudaira, Time-optimal quantum evolution, Phys. Rev. Lett. **96**, 060503 (2006).
[18] J. H. Huang, S. S. Dong, G. L. Chen, N. R. Zhou, F. Y. Liu, and L. G. Qin, Path distance of a quantum unitary evolution, Phys. Rev. A **108**, 022204 (2023).
[19] A. Gilchrist, N. K. Langford, and M. A. Nielsen, Distance measures to compare real and ideal quantum processes, Phys. Rev. A **71**, 062310 (2005).
[20] P. J. Jones and P. Kok, Geometric derivation of the quantum speed limit, Phys. Rev. A **82**, 022107 (2010).
[21] D. Bures, An extension of Kakutani's theorem on infinite product measures to the tensor product of semifinite w*-algebras, Trans. Amer. Math. Soc. **135**, 199 (1969).
[22] W. K. Wootters, Statistical distance and Hilbert space, Phys. Rev. D **23**, 357 (1981).
[23] A. Uhlmann, *Groups and Related Topics* (Kluwer, New York, 1992), pp. 267–274.
[24] S. S. Dong, L. G. Qin, F. Y. Liu, L. H. Gong, and J. H. Huang, Quantum evolution speed induced by Hamiltonian, Acta Phys. Sin. **72**, 220301 (2023).
[25] Y. Z. Wu, J. L. Yuan, C. Y. Zhang, J. F. Deng, Z. T. Zhu, Q. J. Guo, Z. Wang, J. H. Huang, C. Song, H. K. Li, D. W. Wang, H. Wang, and G. S. Agarwal, Testing the unified bounds of the quantum speed limit, arXiv:2403.03579.
[26] L. Mandelstam and I. Tamm, The uncertainty relation between energy and time in non-relativistic quantum mechanics, J. Phys. (Moscow) **9**, 249 (1945).
[27] N. Margolus and L. B. Levitin, The maximum speed of dynamical evolution, Physica D **120**, 188 (1998).
[28] D. P. Pires, M. Cianciaruso, L. C. Celeri, G. Adesso, and D. O. Soares-Pinto, Generalized geometric quantum speed limits, Phys. Rev. X **6**, 021031 (2016).
[29] J. H. Huang, L. Y. Hu, and F. Y. Liu, Instantaneous angular velocity of quantum evolution, Phys. Rev. A **102**, 062221 (2020).

[30] N. Hörnedal, D. Allan, and O. Sönnerborn, Extensions of the Mandelstam-Tamm quantum speed limit to systems in mixed states, New J. Phys. **24**, 055004 (2022).
[31] K. Funo, N. Shiraishi, and K. Saito, Speed limit for open quantum systems, New J. Phys. **21**, 013006 (2019).
[32] F. Q. Dou, M. P. Han, and C. C. Shu, Quantum speed limit under brachistochrone evolution, Phys. Rev. Appl. **20**, 014031 (2023).
[33] N. Il'in and O. Lychkovskiy, Quantum speed limit for thermal states, Phys. Rev. A **103**, 062204 (2021).
[34] G. Ness, A. Alberti, and Y. Sagi, Quantum speed limit for states with a bounded energy spectrum, Phys. Rev. Lett. **129**, 140403 (2022).
[35] T. V. Vu and K. Saito, Topological speed limit, Phys. Rev. Lett. **130**, 010402 (2023).
[36] W. Wu and J. H. An, Quantum speed limit from a quantum-state-diffusion method, Phys. Rev. A **108**, 012204 (2023).
[37] W. Wu and J. H. An, Quantum speed limit of a noisy continuous-variable system, Phys. Rev. A **106**, 062438 (2022).
[38] N. Khaneja, S. J. Glaser, and R. Brockett, Sub-Riemannian geometry and time optimal control of three spin systems: Quantum gates and coherence transfer, Phys. Rev. A **65**, 032301 (2002).
[39] M. A. Nielsen, A geometric approach to quantum circuit lower bounds, Quantum Info. Comput. **6**, 213 (2006).
[40] M. A. Nielsen, M. R. Dowling, M. Gu, and A. C. Doherty, Quantum computation as geometry, Science **311**, 1133 (2006).
[41] V. B. Bulchandani and S. L. Sondhi, How smooth is quantum complexity? J. High Energy Phys. 10 (2021) 230.
[42] V. Balasubramanian, M. DeCross, A. Kar, Y. Li, and O. Parrikar, Complexity growth in integrable and chaotic models, J. High Energy Phys. 07 (2021) 011.
[43] J. M. Magán, Black holes, complexity and quantum chaos, J. High Energy Phys. 09 (2018) 043.
[44] S. Chapman, M. P. Heller, H. Marrochio, and F. Pastawski, Toward a definition of complexity for quantum field theory states, Phys. Rev. Lett. **120**, 121602 (2018).