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Geometric method in quantum control

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In this paper we survey the geometric method in quantum control. By presenting a geometric representation of nonlocal two-qubit quantum operation, we show that the control of two-qubit quantum operations can be reduced to a steering problem in a tetrahedron. Two physical examples are given to illustrate this method. We also provide analytic approaches to construct universal quantum circuit from any arbitrary quantum gate.

quantum control, Cartan decomposition, steering, universal quantum circuit

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Control on quantum mechanical systems has received extensive interests in the past decade due to its fundamental importance in many physical applications of quantum phenomena, e.g., NMR, nanotechnology, molecular systems, quantum optics, and quantum computation [1]. The early research on this topic can be traced back to 1980s. In [2, 3], Tarn et al. investigated modeling and controllability of quantum mechanical control systems. Rabitz et al. discussed optimal control in quantum systems with emphasis on the quantum state transitions [4, 5].

After Shor published his seminal paper on factoring algorithm in mid 1990s [6], quantum system control has attracted particular research efforts as an indispensable part of quantum information processing. The generation of quantum operation is a prerequisite condition for many real physical applications of quantum phenomena. For example, often required in quantum algorithm is to apply Quantum Fourier Transform, which amounts to control the physical system to generate a prescribed quantum operation from initial condition. Other examples include using robust control techniques to protect quantum coherence against environmental noises, and applying quantum feedback control to improve the control performance.

Just as in the case of traditional control, the very first question that quantum system control has to address is how to design open-loop control law. In this paper, we survey the control synthesis technique on generating a desired quantum operation from a given quantum mechanical system. This corresponds to the universality problem in quantum information processing. We consider only discrete variable quantum systems. For continuous variable systems, readers are referred to [7].

Mathematically, a discrete quantum system can be described by quantum states, which are unit vectors in a complex vector space:

$$\{\psi \in \mathbb{C}^N : \|\psi\| = 1\}. \tag{1}$$

When $N = 2$, this corresponds to a 2-dimensional state called a quantum bit, or qubit. A qubit is the simplest quantum system, and it can be used to describe, for example, an electron moving in a magnetic field. A single-qubit state has two basis states denoted as $|0\rangle$ and $|1\rangle$, and any single-qubit state can be expressed as a linear superposition of these two basis states. For an n-qubit state, it contains 2^n basis states, and similar to the single-qubit case, an arbitrary n-qubit state is a linear superposition of its basis states.

To manipulate quantum system, we can apply quantum operations to the quantum state. For an n-qubit system, a quantum gate can be represented by a $2^n \times 2^n$ unitary matrix. Here

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are several single-qubit gates:

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & i \\ -i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

These are indeed the Pauli matrices in quantum physics.

For two-qubit quantum operations, we can distinguish two different types. The first type is local gates, which consists of two single-qubit gates K and L that are applied to an individual qubit. The matrix representation of this local gate is $K \otimes L$, i.e., the tensor product of K and L. Tensor product is also called Kronecker product in control theory. The other type is nonlocal gates, which are the gates that cannot be written as the tensor product of two single-qubit gates. Two important nonlocal gates are CNOT and SWAP gates [8]:

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad \text{SWAP} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

The main problem we consider here is to generate any arbitrary quantum operation from a quantum physical system. This can be treated as a geometric control problem on a Lie group. For the quantum system, the state space is the unitary Lie group that is composed of all the $2^n \times 2^n$ unitary matrices. The dynamics of quantum system is determined by the Schrödinger equation:

$$i\dot{U} = H(v)U, \quad U(t_0) = I. \tag{2}$$

From the perspective of control theory, this is a right invariant vector field on unitary Lie group. Note that the control field v is in the Hamiltonian. Now the generation of quantum gates from quantum system becomes a steering problem, that is, we aim at finding control field v such that the system trajectory generated by Schrödinger equation can achieve the desired target at certain final time.

The control of an n-qubit system is a difficult problem. The reason is threefold. First, the dimension of the problem increases exponentially because the dimension of an n-qubit system is 2^n. Secondly, the dynamics is determined by the bilinear Schrödinger equation. Thirdly, the dynamics is defined on the unitary Lie group, which has complicated group structure.

To simplify this problem, researchers have developed the approach of universal gate set [9]. It is well-known that in classical circuit design NAND is a universal gate because it can be used to implement any arbitrary logic gate. In quantum information processing, the idea is similar. We want to use a set of elementary quantum gates such that any large and complicated quantum gate can be decomposed as a combination of these elementary gates. The standard result in the literature is that any quantum gate on arbitrarily many qubits can be decomposed as a composition of single- and two-qubit gates. Therefore, to implement any arbitrary quantum gate, we need to implement only single- and two-qubit gates. The single-qubit gates are defined on the Lie group $SU(2)$. The control of $SU(2)$ is the same as that of $SO(3)$, the rotation matrix group, because $SU(2)$ is a double cover of $SO(3)$. This is a well-studied problem in many other disciplines such as robotics [10], and its extension to one-qubit gates has been studied in details in, e.g., [11].

In the rest of this paper, we will thus assume that the single-qubit gates can be readily generated, and we will focus on the implementation of two-qubit gates, which is a control problem on the Lie group $SU(4)$.

1 Basic control strategy

We first give a brief introduction about the mathematical background of the control problems on $SU(4)$, the set of all the two-qubit quantum operations.

The Lie algebra $\mathfrak{su}(4)$ has a direct sum decomposition $\mathfrak{su}(4) = \mathfrak{k} \oplus \mathfrak{p}$, where

$$\begin{aligned} \mathfrak{k} &= \text{span}\, \frac{i}{2}\{\sigma_x^1, \sigma_y^1, \sigma_z^1, \sigma_x^2, \sigma_y^2, \sigma_z^2\}, \\ \mathfrak{p} &= \text{span}\, \frac{i}{2}\{\sigma_x^1\sigma_x^2, \sigma_x^1\sigma_y^2, \sigma_x^1\sigma_z^2, \sigma_y^1\sigma_x^2, \sigma_y^1\sigma_y^2, \sigma_y^1\sigma_z^2, \\ &\qquad \sigma_z^1\sigma_x^2, \sigma_z^1\sigma_y^2, \sigma_z^1\sigma_z^2\}. \end{aligned} \tag{3}$$

Here σ_x, σ_y, and σ_z are the Pauli matrices, and $\sigma_\alpha^1\sigma_\beta^2 = \sigma_\alpha \otimes \sigma_\beta$. From the Lie bracket computation, it is easy to obtain that

$$[\mathfrak{k}, \mathfrak{k}] \subset \mathfrak{k}, \quad [\mathfrak{p}, \mathfrak{k}] \subset \mathfrak{p}, \quad [\mathfrak{p}, \mathfrak{p}] \subset \mathfrak{k}. \tag{4}$$

Therefore $\mathfrak{su}(4) = \mathfrak{k} \oplus \mathfrak{p}$ is a Cartan decomposition, and any $U \in SU(4)$ can be decomposed as

$$U = k_1 A k_2 = k_1 \exp\{\frac{i}{2}(c_1\sigma_x^1\sigma_x^2 + c_2\sigma_y^1\sigma_y^2 + c_3\sigma_z^1\sigma_z^2)\}k_2, \tag{5}$$

where $k_1, k_2 \in SU(2) \otimes SU(2)$, and $c_1, c_2, c_3 \in \mathbb{R}$.

Our basic control strategy to generate any arbitrary two-qubit operation is to separate the implementation of one- and two-qubit gates. To explain this idea, we need to introduce the notion of local equivalence. Two unitary transformations U, $U_1 \in SU(4)$ are called local equivalent if they differ only by local operations: $U = k_1 U_1 k_2$, where k_1, $k_2 \in SU(2) \otimes SU(2)$ are local gates. We denote this equivalence relation as $U \sim U_1$, and the equivalence class of U as $[U]$. It can be easily proved that this local equivalence relation defines an equivalence class on the whole space of all the two-qubit quantum operations. Now remember we assume all the 1-qubit gate can be implemented. Therefore, to implement a two-qubit gate U, we only need to implement a gate U_1 that is locally equivalent to U. Once we obtain U_1, we can just add on those two local gates k_1 and k_2 to achieve U exactly. Therefore, our original control problem on the unitary Lie group becomes a control problem on the local equivalence classes.

Before we can solve the control on the equivalence classes, we need to answer the following two questions:

(1) Given two gates U and U_1, how to determine whether or not they are locally equivalent?

(2) What is the structure of local equivalence classes?

The first question was answered by Makhlin in [13], where a procedure was given to calculate two local invariants G_1 and G_2. The assertion is that if two-qubit operations U and U_1 are locally equivalent to each other if and only if they have identically the same local invariants. We include this procedure here for completeness. For a given two-qubit gate U, define $U_B = Q^\dagger U Q$, where

$$Q = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 0 & 0 & i \\ 0 & i & 1 & 0 \\ 0 & i & -1 & 0 \\ 1 & 0 & 0 & -i \end{pmatrix}. \tag{6}$$

Let $m = U_B^T U_B$. Then the local invariants are given by

$$G_1 = \frac{\text{trace}^2\,(m(U))}{16 \det U}, \tag{7}$$

$$G_2 = \frac{\text{trace}^2\,(m(U)) - \text{trace}\,(m^2(U))}{4 \det U}. \tag{8}$$

In the following table, we list the local invariants for several commonly-used two-qubit gates.

	G_1	G_2
Local gates	1	3
CNOT	0	1
C(Z)	0	1
SWAP	−1	−3

It is evident that CNOT and Controlled-Z (referred as C(Z)) are locally equivalent because they possess identical local invariants $G_1 = 0$ and $G_2 = 1$.

To answer the second question, we insert Cartan decomposition (5) into Makhlin's procedure and obtain that [14]

$$\begin{aligned} G_1 &= \cos^2 c_1 \cos^2 c_2 \cos^2 c_3 - \sin^2 c_1 \sin^2 c_2 \sin^2 c_3 \\ &\quad + \frac{i}{4} \sin 2c_1 \sin 2c_2 \sin 2c_3, \\ G_2 &= 4\cos^2 c_1 \cos^2 c_2 \cos^2 c_3 - 4\sin^2 c_1 \sin^2 c_2 \sin^2 c_3 \\ &\quad - \cos 2c_1 \cos 2c_2 \cos 2c_3. \end{aligned} \tag{9}$$

Eq. (9) unravels the relation between the local invariants G_1 and G_2 and the coordinates $[c_1, c_2, c_3]$ of a two-qubit gate. From this relation, given a triplet $[c_1, c_2, c_3]$, we can easily compute the local invariants; and vice versa, from a given pair of local invariants G_1 and G_2, we can also find the corresponding triplet. The real space $\mathbb{R}^3$ thus provides a geometric representation of local equivalence classes. However, this representation is not unique, as we can find multiple points in $\mathbb{R}^3$ that correspond to the same local equivalence class. We need to remove the redundancy in this representation.

After examining eq. (9), we have the following observations:

(1) Periodicity: $[c_1, c_2, c_3] \sim [c_1+m_1\pi, c_2+m_2\pi, c_3+m_3\pi]$;

(2) Symmetry:

Permutation: $[c_1, c_2, c_3] \sim [c_3, c_2, c_1]$;

Sign flips: $[c_1, c_2, c_3] \sim [-c_1, c_2, -c_3]$.

From periodicity, we can cut down the redundancy and visualize the geometric structure of the two-qubit gates as a cube with side length π in $\mathbb{R}^3$ as shown in Figure 1(a). This provides an equivalent representation of the points on the 3-Torus, since $T^3 \cong \mathbb{R}^3/\mathbb{Z}^3$. Every point in this cube corresponds to a local equivalence class, yet different points in the cube may belong to the same local equivalence class.

To further remove the redundancy, we notice that the symmetric points correspond to those points that are reflections of each other with respect to some diagonal planes in the cube. We can cut along these diagonal planes, and the resulting two pieces contain the same local equivalence classes. We can thus discard one of them. After this procedure, we obtain a tetrahedral representation of local equivalence classes of two-qubit as shown in Figure 1(b). Note that for any point $[c_1, c_2, 0]$ on the base of this tetrahedron, its mirror image with respect to the line LA_2, which is $[\pi - c_1, c_2, 0]$, corresponds to the same local equivalence class. Therefore, with the caution that the basal areas LA_2A_1 and LA_2O are identified together, we obtain a geometric representation of local equivalence classes. This is also called Weyl chamber in the Lie group representation theory [12].

In Figure 1(b), the local gates correspond to the points O and A_1, and CNOT is L, SWAP is A_3, and Controlled-U gates are the line OL.

2 Steering in the tetrahedron

With the geometric representation of local equivalence classes, we can use the steering in the tetrahedron to generate any arbitrary two-qubit operation.

The general idea is as follows. For a given quantum system whose dynamics is determined by the Schrödinger equation in eq. (2), control field v will generate a trajectory in the state

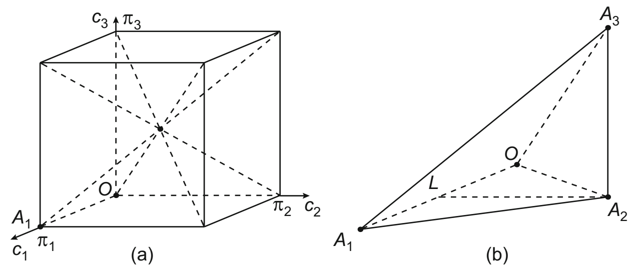


Figure 1 Tetrahedral representation of nonlocal two-qubit operations. (a) Cubic representation. (b) Tetrahedron representation: every point corresponds to a local equivalence class of two-qubit operations.

space $U(4)$. At any time instant t, $U(t)$ is a point on that trajectory. From Makhlin's procedure, we can calculate local invariants from $U(t)$ as $G_1(U(t))$ and $G_2(U(t))$. Then from eq. (9), we can locate a point $[c_1(t), c_2(t), c_3(t)]$ in the tetrahedron. As time evolves, we can obtain a continuous trajectory. Now if our control target is to generate a quantum operation, say CNOT, we can first find the control field v that drives the trajectory in the tetrahedron to hit the point L. Since we have implemented a gate that is locally equivalent to CNOT, what is left is just to add on two local gates that we assumed can be implemented readily. This is the idea of steering in the tetrahedron.

We illustrate the idea by the following two examples.

Example 2.1. Consider a purely nonlocal Hamiltonian

$$H = -\frac{1}{2}(c_x\sigma_x^1\sigma_x^2 + c_y\sigma_y^1\sigma_y^2 + c_z\sigma_z^1\sigma_z^2). \tag{10}$$

For constant control fields c_x, c_y, and c_z, the quantum operations generated by this Hamiltonian can be written as

$$U(t) = \exp(-iHt) = \exp\frac{i}{2}(c_xt\sigma_x^1\sigma_x^2 + c_yt\sigma_y^1\sigma_y^2 + c_zt\sigma_z^1\sigma_z^2).$$

It thus yields a trajectory $[c_x, c_y, c_z]t$ in the tetrahedron, which is a straight line. We can apply certain gate from a finite group of local operations (dubbed as Weyl group [14]) to change the evolution direction of this trajectory. This indeed corresponds to the reflection with respect to some diagonal plane of the cube in Figure 1(a). Then we can obtain new directions such as $[c_x, -c_y, -c_z]t$, $[-c_x, c_y, -c_z]t$, and $[c_x, c_z, c_y]t$. Piecing together two such trajectories, we can get a quantum operation, e.g.,

$$e^{\frac{i}{2}\sigma_x^1\pi}\cdot\exp(-iHt_2)\cdot e^{-\frac{i}{2}\sigma_x^1\pi}\cdot\exp(-iHt_1),$$

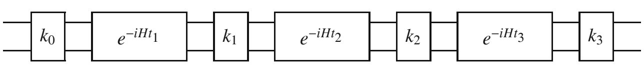
whose endpoint can be written as

$$[c_x, -c_y, -c_z]t_2 + [c_x, c_y, c_z]t_1.$$

We can thus achieve anywhere in the plane OA_1A_2. If changing direction twice, we can arrive any arbitrary point in the tetrahedron.

We then have the following result [14].

Proposition 2.2. For a pure nonlocal Hamiltonian, the following quantum circuit can implement any two-qubit gate.



Example 2.3. Consider an isotropic exchange with local terms

$$H = (g_1\cdot\vec{\sigma})\otimes I + I\otimes(g_2\cdot\vec{\sigma}) + J(\sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2 + \sigma_z^1\sigma_z^2), \tag{11}$$

where g_1, $g_2 \in \mathbb{R}^3$, and $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$. This Hamiltonian can be used to describe, e.g., spin-coupled quantum dots [15, 16]. We can tune the single-qubit control fields g_1 and g_2 to be parallel, that is, $g_1 = \alpha g_2$, where α characterizes the ratio. In this case, the tetrahedral trajectory is given by

$$c_1(t) = 2Jt,$$
$$c_2(t) = c_3(t) = \left|\sin^{-1}\left(\frac{2J}{\omega}\sin\omega t\right)\right|,$$

where $\omega = \sqrt{(\|g_1\| - \|g_2\|)^2 + 4J^2}$. We can implement CNOT by choosing $2Jt = \frac{\pi}{2}$ and $\omega t = k\pi$. One particular choice of control parameters can be given as

$$k = 4,\ t = 2.5\pi,\ g_1 = [4, 4, 4],\ g_2 = [3, 3, 3]. \tag{12}$$

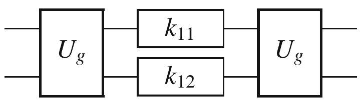
The corresponding tetrahedral trajectory is shown in Figure 2.

3 Quantum circuit construction

In this section we consider the problem of generating any two-qubit operation from a given two-qubit gate U_g and local gates. This is closely related to the control problem discussed earlier, and can be another example illustrating the application of tetrahedral representation of nonlocal gates.

The motivation is that in many physical situations the Hamiltonian is unknown; or the Hamiltonian is known, but it can be switched on for only a fixed amount of time, e.g., in encoded quantum systems [17]. Under these circumstances, we are given a specific two-qubit operation, and we want to construct any arbitrary operation from this given gate together with local gates.

We now review some results from [18]. The first step in the construction is to implement a Controlled-U gate from two applications of U_g:



Recall that the Controlled-U gates are located on the line OA_1. We can then use the Controlled-U as a basic building block to generate any desired two-qubit gate. Interested readers may find the detailed analytical procedure in [18].

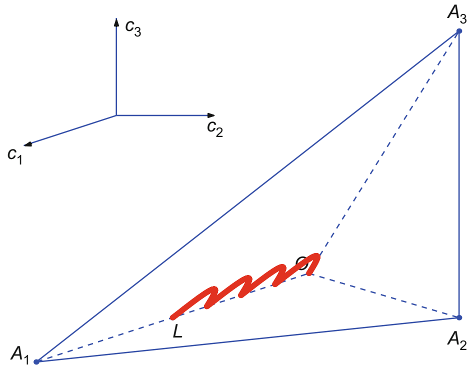


Figure 2 (Color online) Tetrahedral trajectory generated by the Hamiltonian in eq. (11) with parameters (12).

One particularly interesting problem is the efficiency of Controlled-U, that is, for a given Controlled-U gate $U_g = e^{\gamma \frac{i}{2}\sigma_x^1\sigma_x^2}$, how many applications do we need to construct any arbitrary two-qubit operation? By Kostant's convexity theorem, we can prove that the minimum number required is given by

$$n_{\min} = \left\lceil \frac{3\pi}{2\gamma} \right\rceil.$$

In Figure 3, we plot the minimum upper bound for U_g to construct any two-qubit gate as a function of γ. It is clear that the most efficient Controlled-U is when $\gamma = \frac{\pi}{2}$, which is none other than the CNOT gate. Analytical results can be obtained to construct a universal quantum circuit from CNOT by three applications. Probing further, we find that DCNOT given below is equally efficient

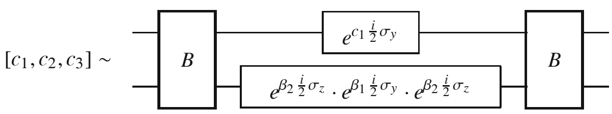
$$\exp\left\{\frac{i}{2}\left(\frac{\pi}{2}\sigma_x^1\sigma_x^2 + \frac{\pi}{2}\sigma_y^1\sigma_y^2\right)\right\},$$

as it can generate any two-qubit gate by three applications as well.

Note that DCNOT is not a Controlled-U gate, which leads us to wonder what is the most efficient universal gate among all the two-qubit operations. The answer is a gate that we named as the B gate:

$$B = \exp\left\{\frac{i}{2}\left(\frac{\pi}{2}\sigma_x^1\sigma_x^2 + \frac{\pi}{4}\sigma_y^1\sigma_y^2\right)\right\}.$$

The significance of the B gate is that with only two applications it can generate any two-qubit operation:



where the parameters β_1 and β_2 are determined by c_2 and c_3 in a closed-form solution.

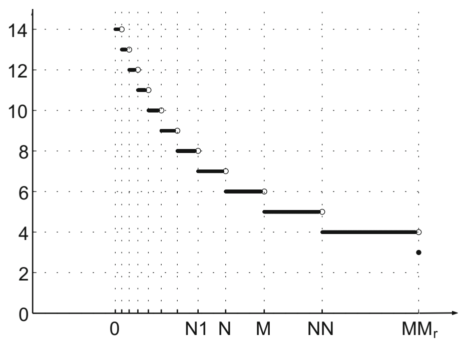


Figure 3 Minimum upper bound of applications required for $U_g = e^{\gamma \frac{i}{2}\sigma_x^1\sigma_x^2}$ to construct an arbitrary two-qubit gate.

4 Summary

In this paper we reviewed the geometric method in the control of quantum mechanical system. We discussed that a generic open-loop state transfer control is equivalent to the universality problem in quantum information processing. We presented a geometric representation of two-qubit quantum operations, and showed that a control problem on two-qubit system can be converted into a steering problem in a tetrahedron. Two physical examples are given to illustrate this approach. We then studied analytic solutions to generate quantum operations from a generic quantum gate, and investigated the efficiency in the construction of universal quantum circuit.

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