

Generation of quantum logic operations from physical Hamiltonians

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We provide a systematic analysis of the physical generation of single- and two-qubit quantum operations from Hamiltonians available in various quantum systems for scalable quantum information processing. We show that generation of single-qubit operations can be transformed into a steering problem on the Bloch sphere, which represents all R_z -equivalence classes of single-qubit operations, whereas the two-qubit problem can be generally transformed into a steering problem in a tetrahedron representing all the local-equivalence classes of two-qubit operations (the Weyl chamber). We use this approach to investigate several physical examples for the generation of two-qubit operations. The steering approach provides useful guidance for the realization of various quantum computation schemes.

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I. INTRODUCTION

Physical implementation of quantum information processing and quantum computation usually begins with a coupled quantum mechanical system and requires that the available Hamiltonian for that system be controlled to generate the desired quantum operations from which the quantum algorithm is constructed [1,2]. It is therefore a fundamental issue to produce quantum operations from the Hamiltonian that is provided by or accessible to the physical quantum system. In this work we formulate the generation of these operations as a problem in control theory and show that this language is beneficial to developing efficient physical implementation of quantum operations for computation and information processing.

The postulates of quantum mechanics assert that the state of a quantum system is completely described, at time t , by a unit vector $|\psi(t)\rangle$ in a Hilbert space [3]. The evolution of $|\psi(t)\rangle$ is determined by $|\psi(t)\rangle = U(t)|\psi(0)\rangle$, where $U(t)$ is a unitary evolution operator (or propagator). The dynamics of $U(t)$ is given by Schrödinger's equation $i\hbar\dot{U}(t) = H(v)U(t)$ with $U(0) = I$, where H is the Hamiltonian of the system and v the external control field. The generation of quantum operation means to find a control v such that the trajectory generated by Schrödinger's equation can achieve a prescribed target unitary operator U_T at certain final time. This can be posed as a steering problem in control theory. The state space of this control system is the unitary Lie group $U(2^n)$, which consists of all the quantum operations on the n -qubit system, and the dynamics of quantum operation described by Schrödinger's equation is a right-invariant vector field on the unitary Lie group $U(2^n)$.

Steering on Lie groups has been studied for a long time, and it still remains a very difficult problem in control theory [4]. It is well known that when the control distribution is bracket generating, the system is controllable; i.e., there exists a control law that steers the system from any initial state to any final state in the state space [5,6]. Nevertheless, this result does not provide a constructive way to find the control law. One useful mathematical tool to solve the steering prob-

lem is to use Pontryagin's maximum principle, which gives a set of differential equations that have to be satisfied by the optimal trajectory [7–10]. Quite often, however, this approach leads to a two-point fixed-boundary problem which has no analytic solutions [11].

In this paper, we develop a general approach to design the control law for generation of an arbitrary quantum operation from the available Hamiltonians in quantum mechanical systems. Because any quantum operation on any arbitrary large quantum system can be decomposed as a combination of single- and two-qubit quantum operations [1], we only need to study the control of single two-level systems and pairs of coupled two-level systems, which amounts to the steering problem on the unitary Lie groups $U(2)$ and $U(4)$, respectively. The key idea of the approach here is based on the observation that in many real quantum systems there exists a certain subset of quantum operations that can be readily generated. This observation leads naturally to the notion of control on a quotient space; that is, instead of controlling the original high-dimensional complicated quantum system, we study a reduced control problem on a quotient space obtained from an equivalence relation that is defined for two quantum operations if they differ only by quantum operations in that specific subset. Therefore, to generate a desired target quantum operation, we can equivalently generate a quantum operation that differs from the target by a quantum operation in the easily achieved subset. One key issue in this approach is to find the structure of the quotient space and the reduced control trajectory on this quotient space. This makes it possible to study the generation of quantum operations by solving a steering problem on the quotient space. We present solutions here for steering on the quotient space of both $U(2)$ and $U(4)$. The solutions for $U(2)$ are related to those known from the NMR literature, but are developed here in a unified steering framework that also encompasses the solutions for the more complex $U(4)$.

We start with the generation of single-qubit operations, which can be viewed as a control problem on a two-level system. We know that all the single-qubit operations form the unitary Lie group $U(2)$ and that any single-qubit operation can be described as a rotation on the Bloch sphere of a

certain angle about a specified axis. In many two-level quantum systems, it is often easy to generate a rotation operator $R_{\hat{n}}$ about a fixed axis \hat{n} by appropriate choice of a static control field. By making a change of coordinates one can transform $R_{\hat{n}}$ into R_z —i.e., the rotation operator about the z axis. Consequently, to implement an arbitrary single-qubit quantum operation U_T , we only need to implement a quantum operation \tilde{U}_T that differs from U_T by a z rotation operator from the right—that is, $U_T = \tilde{U}_T R_z(\theta)$, with $\theta \in [0, 2\pi)$. This defines an equivalence relation on all the single-qubit quantum operations, and the quotient space obtained from this equivalence relation is nothing but the Bloch sphere. Therefore, the generation of arbitrary single-qubit operations can be transformed to a steering problem on the Bloch sphere combined with a single rotation about the z axis. For the case when the control is an oscillating field perpendicular to the static field, we derive the control laws for generation of arbitrary single-qubit operations that are familiar from the NMR literature. We also prove that the system is controllable if and only if the oscillating field is tuned at the resonant frequency. We then study the case when the oscillating field is not perpendicular to the static field. For both of these two cases, we show that when at resonant frequency, the total time to implement a given operation is quantized. This is a particularly important issue for the implementation of local unitary operations in coupled two-qubit systems, for which two single-qubit operations must be generated at the same time. We also show that when the control variable is varied within a certain range, an efficient way to generate any single-qubit operation is to simply alternate between the two extremal values of the control parameter. A control law design based on the Bloch sphere steering technique thus provides a complete solution to the generation of any arbitrary local unitary operations from a given Hamiltonian.

We then consider the generation of two-qubit quantum operations. Physically, this is a control problem on two coupled two-level systems. It is much more difficult to control a coupled qubit system to generate the desired two-qubit quantum operation, because of the higher dimensionality and more complicated Lie group structure. In Ref. [10], Khaneja *et al.* derived the time-optimal solution when the Hamiltonian is purely nonlocal. However, when the Hamiltonian contains both local and nonlocal terms with comparable magnitudes, there are no systematic methods to derive the control laws other than numerical procedures [12,13]. In this paper, we provide a systematic approach to solve this problem by using the notion of control on a quotient space. Our control strategy employs two steps to generate an arbitrary two-qubit operation U_T . First, we find an efficient control law to generate a nonlocal quantum operation U_1 that differs from U_T only by local unitary operations k_1 and k_2 , where each of these is the tensor product of two single-qubit quantum operations. Then we consider generation of the local operations k_1 and k_2 , which is required in order to arrive at U_T in the computational basis. This will often require that the single-qubit operations be implemented simultaneously (see above).

A basic principle in this control design strategy is that we implement the local and two-qubit operations separately.

This is often feasible in many physical applications, where the single-qubit operations are generated by local Hamiltonians that can be independently controlled—e.g., by external fields—so that we can readily implement any local unitary operation. This separation leads naturally to the concept of local equivalence on all two-qubit quantum operations [14]. In Ref. [15], we derived the geometric representation of this equivalence relation as a tetrahedron, referred to as the Weyl chamber. Each point in the tetrahedron represents a local-equivalence class of some nonlocal two-qubit operations. The generation of a two-qubit quantum operation can then be treated as a steering problem in this tetrahedron. We have shown some examples of this steering technique [15], when the Hamiltonian is given in some special cases—e.g., purely nonlocal. In this paper, we will exploit this idea to more systematically study the generation of two-qubit operations for a variety of Hamiltonians that include both nonlocal and local terms and that derive from physical systems relevant to implementation of quantum information processing, in particular to solid-state implementations.

II. GENERATION OF SINGLE-QUBIT OPERATIONS: STEERING ON THE BLOCH SPHERE

In this section, we study the generation of single-qubit operations as a control problem of unitary transformations on two-level quantum systems. The time evolution operator for a general two-level system can be written as follows:

$$i\dot{U} = (H_d + vH_c)U, \quad U(0) = I, \quad (1)$$

where H_d is the drift Hamiltonian, H_c the control Hamiltonian, and v the control. Here H_d and H_c are both Hermitian matrices on $\mathbb{C}^{2 \times 2}$. Upon neglecting the global phase term, all single-qubit quantum operations form a Lie group $SU(2)$:

$$SU(2) = \{U \in \mathbb{C}^{2 \times 2} : UU^\dagger = I, \det U = 1\}.$$

Our task is to find the control v that will drive the system (1) from the initial operation $U(0)=I$ to a prescribed target quantum operation U_T . Note that we have implicitly subdivided the physical Hamiltonian into a term that cannot be varied, H_d , and a term that may be controlled externally, H_c .

To solve this control problem, we first transform Eq. (1) into the following standard form:

$$i\dot{U} = (a\sigma_z + vH_c)U. \quad (2)$$

This transformation is obtained by the following argument. Without loss of generality, we can assume that $H_d = a_1\sigma_x + a_2\sigma_y + a_3\sigma_z$, where σ_x , σ_y , and σ_z are Pauli matrices. When $a_1^2 + a_2^2 \neq 0$, let

$$k = \begin{pmatrix} \frac{a_1 - a_2i}{\sqrt{2a(a - a_3)}} & \frac{-a_1 + a_2i}{\sqrt{2a(a + a_3)}} \\ \sqrt{\frac{a - a_3}{2a}} & \sqrt{\frac{a + a_3}{2a}} \end{pmatrix},$$

where $a = \sqrt{a_1^2 + a_2^2 + a_3^2}$. It is straightforward to verify that $kk^\dagger = I$; i.e., k is a single-qubit operation. One can also verify

that $kH_d k^{-1} = a\sigma_z$. Then, letting $U_1 = kU$, we have

$$i\dot{U}_1 = k(H_d + vH_c)k^{-1}U_1 = (a\sigma_z + vkH_c k^{-1})U_1,$$

where we have recognized that $kH_c k^{-1} = H'_c$, which puts this into the form of Eq. (2). The original control problem of steering Eq. (1) from $U(0) = I$ to U_T is thereby transformed into a problem of steering Eq. (2) from $U_1(0) = k$ to kU_T . For control of a single qubit, we therefore only need to consider the standard form (2).

A. Steering on the Bloch sphere

If no control signals are applied—i.e., $v=0$ —Eq. (2) simplifies to

$$i\dot{U} = a\sigma_z U. \quad (3)$$

The solution to Eq. (3) is simply the σ_z rotation operator $R_z(2at) = e^{-ia\sigma_z t}$. We can thus easily implement any σ_z rotation by turning off the control v and letting the system evolve for a certain time duration under H_d alone.

We now introduce the notion of R_z equivalence and show that it provides a simple and intuitive approach to derive the control fields required to implement an arbitrary single-qubit quantum operation without loss of generality. Two single-qubit operations U_T and \tilde{U}_T are R_z equivalent if they satisfy

$$U_T = \tilde{U}_T e^{-i\sigma_z t_z}. \quad (4)$$

It is evident that this relation is reflexive, symmetric, and transitive, and therefore it is an equivalence relation on the Lie group $SU(2)$ of all the single-qubit operations. A general procedure to implement an arbitrary single-qubit operation is then to first generate a rotation about the z axis for a finite time duration t_z , with $v=0$ as described above, and then to steer on the quotient space of all the R_z -equivalence classes with an external control $v \neq 0$ chosen to drive the system to an operation \tilde{U}_T that is R_z equivalent to U_T .

We now show that this quotient space is nothing but the Bloch sphere. Recall that the state of a single qubit can be represented by $|\psi\rangle = z_1|0\rangle + z_2|1\rangle$, where z_i are complex numbers with the restriction $|z_1|^2 + |z_2|^2 = 1$. Ignoring the global phase, this state can be written as

$$|\psi\rangle = \cos\frac{\theta}{2}|0\rangle + e^{i\phi}\sin\frac{\theta}{2}|1\rangle,$$

where the real numbers θ and ϕ define a point $(x, y, z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta)$ on a unit sphere, which is the well-known *Bloch sphere* shown in Fig. 1. To find θ and ϕ explicitly, we can use the Hopf fibration, which is a map $\pi: S^3 \rightarrow S^2$ defined by $\pi(\psi) = (x, y, z) \in S^2$ [16], with

$$(z, x + yi) = (|z_1|^2 - |z_2|^2, 2\bar{z}_1 z_2). \quad (5)$$

We define a map Φ from a single-qubit operation to a point on the Bloch sphere by $\Phi(U) = U|1\rangle$, where $|1\rangle$ is the single-qubit state corresponding to the south pole of the Bloch sphere. Then

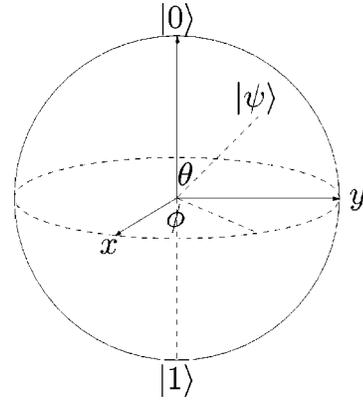


FIG. 1. Bloch sphere representation of a single qubit.

$$\Phi(e^{-ia\sigma_z t}) = e^{-ia\sigma_z t}|1\rangle = |1\rangle.$$

Furthermore, if U_T and \tilde{U}_T are R_z equivalent, we have $\Phi(U_T) = \Phi(\tilde{U}_T)$. Therefore, all operations that are R_z equivalent are mapped to the same point on the Bloch sphere. Conversely, it can also be proved by Lie group theory [16] that all operations that are mapped to the same point on the Bloch sphere differ only by a σ_z rotation from the right; that is, they are all R_z equivalent. We thereby obtain that the quotient space of R_z equivalence classes on $SU(2)$ can be represented by the Bloch sphere.

Now our control task becomes a steering problem on the Bloch sphere that can be accomplished by v . Under the above mapping, the initial point of this steering problem is $\Phi(I) = |1\rangle$ and the final point is $U_T|1\rangle$, where U_T is the desired target operation. The form of the control v that can generate a trajectory on the Bloch sphere reaching the final point $U_T|1\rangle$ from the initial point $|1\rangle$ will depend on the nature of the control Hamiltonian H_c . We emphasize that this Bloch sphere steering follows an initial z -axis rotation for finite time t_z and that the combination of these two steps thereby allows the construction of an arbitrary $SU(2)$ operation. In the remaining part of this section, we illustrate this strategy with three examples.

B. Oscillating control field

We illustrate this approach of control on the quotient space with an analysis of the generation of single-qubit operations on two-level quantum systems subject to an oscillating electromagnetic control field $A/2 \cos(\omega t + \delta)$. Some of the results shown below are known within the NMR literature, in particular that for a control field perpendicular to the static field. However, the solutions look different because the analysis here is made in the laboratory frame, instead of in a rotating frame as is customary in the NMR community. In NMR, under the usual operating conditions the coupling terms simplify to an Ising interaction which is invariant under the rotating frame transformation. In the general case, when the coupling term is not of the Ising form, a time-independent coupling Hamiltonian in the laboratory frame will be time dependent in the rotating frame. As noted above, implementation of a two-qubit local gate—i.e.,

$k_1 = k_{11} \otimes k_{12}$ —requires simultaneous implementation of each single-qubit operation k_{11} and k_{12} . We show below that such simultaneous single-qubit operations are readily steered in the laboratory frame. The same argument applies to local gates in larger multiqubit arrays.

1. Perpendicular control field

We first consider the case in which the control Hamiltonian H_c is an oscillating control field perpendicular to a static drift field H_d . This is prevalent in many quantum systems: e.g., electron spin resonance (ESR). Here a single atom

is placed in a uniform constant magnetic field directed along the z axis, and the control is an oscillating magnetic field oriented along the x axis [17]. The dynamics of the quantum spin is determined by

$$i\dot{U} = \left(\frac{\omega_0}{2} \sigma_z + \frac{A}{2} \cos(\omega t + \delta) \sigma_x \right) U. \quad (6)$$

A solution to Eq. (6) for near resonance, $\omega \sim \omega_0$, may be found by transforming first to a rotating frame defined by the drift (Larmor) frequency—i.e., $U_1 = e^{i\omega_0 t/2} \sigma_z U$. We then obtain

$$i\dot{U}_1 = \frac{A}{2} \cos(\omega t + \delta) (\sigma_x \cos \omega_0 t - \sigma_y \sin \omega_0 t) U_1 = \frac{A}{4} \begin{pmatrix} 0 & e^{i[(\omega+\omega_0)t+\delta]} + e^{-i[(\omega-\omega_0)t+\delta]} \\ e^{-i[(\omega+\omega_0)t+\delta]} + e^{i[(\omega-\omega_0)t+\delta]} & 0 \end{pmatrix} U_1.$$

Since for near resonance between drift and control fields the terms $e^{\pm i[(\omega+\omega_0)t+\delta]}$ oscillate much faster than the terms $e^{\pm i[(\omega-\omega_0)t+\delta]}$, they make on average little contribution to \dot{U}_1 and can be neglected (rotating-wave approximation), resulting in the approximate equation

$$i\dot{U}_1 = \frac{A}{4} (\cos[(\omega - \omega_0)t + \delta] \sigma_x + \sin[(\omega - \omega_0)t + \delta] \sigma_y) U_1. \quad (7)$$

Now letting $U_2 = e^{i[(\omega-\omega_0)t+\delta]/2} \sigma_z U_1$, we have

$$i\dot{U}_2 = \left(\frac{A}{4} \sigma_x + \frac{\omega_0 - \omega}{2} \sigma_z \right) U_2, \quad (8)$$

which has an explicit solution

$$U_2(t) = e^{-i[A/4 \sigma_x + (\omega_0 - \omega)/2 \sigma_z] t}.$$

Combining these two transformations, we obtain an approximate solution (i.e., within the rotating-wave approximation) to Eq. (6) as

$$U(t_f) = e^{-i(\omega t_f + \delta)/2} \sigma_z e^{-i[A/4 \sigma_x + (\omega_0 - \omega)/2 \sigma_z] t_f} e^{i\delta/2} \sigma_z. \quad (9)$$

This is equivalent to the standard treatment of ESR and NMR [17]. Since we can also generate any σ_z rotation by turning off the control field H_c for a time duration t_z , a general form of the quantum operation generated by this system can then be written as

$$\begin{aligned} U(t_f, t_z) &= U(t_f) e^{-i\omega_0/2} \sigma_z t_z \\ &= e^{-i(\omega t_f + \delta)/2} \sigma_z e^{-i[A/4 \sigma_x + (\omega_0 - \omega)/2 \sigma_z] t_f} e^{i(\delta - \omega_0 t_z)/2} \sigma_z. \end{aligned} \quad (10)$$

In the language of control on the quotient space developed above, the effect of the operation $U(t_f, t_z)$ on the quantum state $|1\rangle$ can be described directly from Eq. (10) as a rotation about the axis $(A/2, 0, \omega_0 - \omega)$ followed by another rotation about the z axis, as shown in Fig. 2 for both near-

resonant (A) and resonant (B) situations. From this it is evident that when $\omega \neq \omega_0$, all points (x, y, z) on the Bloch sphere satisfying

$$z \geq \frac{(A/2)^2 - (\omega_0 - \omega)^2}{(A/2)^2 + (\omega_0 - \omega)^2}, \quad (11)$$

shown as the shaded area in Fig. 2, can never be reached for any choice of tuning parameters A, δ and time durations t_f, t_z . Consequently, the reachable set in this near-resonant case is not *all* single-qubit operations. To allow implementation of any arbitrary single-qubit operation, we must impose the strict condition $\omega = \omega_0$; that is, the oscillating field must be tuned to the resonant frequency.

We now show that when operating at exact resonance, the time duration to implement an arbitrary single-qubit rotation in the laboratory frame is quantized. At resonance, Eq. (10) becomes

$$U(t_f, t_z) = e^{-i(\omega_0 t_f + \delta)/2} \sigma_z e^{-iA/4 \sigma_x t_f} e^{i(\delta - \omega_0 t_z)/2} \sigma_z. \quad (12)$$

On the other hand, we know from Euler's ZZZ decomposition that an arbitrary single-qubit operation U_T can be decomposed as

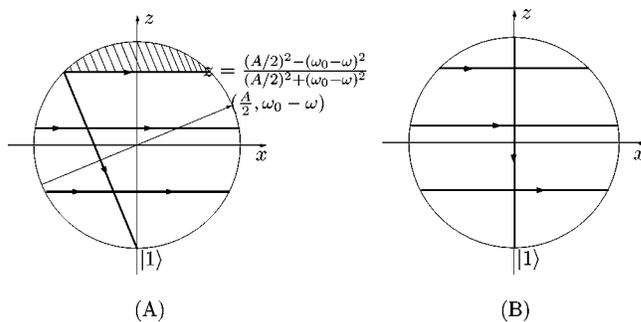


FIG. 2. The effect of the single-qubit operation $U(t_f, t_z)$, Eq. (10), on the quantum state $|1\rangle$: (A) $\omega \neq \omega_0$ and (B) $\omega = \omega_0$.

$$U_T = e^{-i(\phi-\pi/2)/2\sigma_z} e^{-i(\pi-\theta)/2\sigma_x} e^{-i\gamma/2\sigma_z}. \quad (13)$$

Note that in Eq. (13) the coefficients in the first two terms are chosen such that U_T is mapped to the point (θ, ϕ) on the Bloch sphere. Comparing Eqs. (12) and (13), we find that for $\omega = \omega_0$, an arbitrary single-qubit operation U_T in Eq. (13) can be implemented if the following conditions are satisfied:

$$\phi - \pi/2 + 2m_1\pi = \omega_0 t_f + \delta, \quad (14)$$

$$\pi - \theta + 2m_2\pi = \frac{A}{2} t_f, \quad (15)$$

$$-\gamma + 2m_3\pi = \delta - \omega_0 t_z, \quad (16)$$

where $m_1, m_2, m_3 \in \mathbb{Z}$ and $m_1 + m_2 + m_3$ is even. Any values of the control parameters A and δ and time durations t_z and t_f that satisfy Eqs. (14)–(16) can generate the desired target operation U_T within the total time $t_f + t_z$. From Eqs. (14) and (16), we also find that

$$t_f + t_z = \frac{\phi + \gamma - \pi/2 + 2m\pi}{\omega_0}, \quad (17)$$

where m is an integer. Hence, from Eq. (17), it is evident that if the oscillating field is tuned at resonant frequency, the time duration to implement a single-qubit operation is quantized with a time duration that is independent of the amplitude of the oscillating control field. This is a particularly important issue in the generation of two-qubit local unitary operations, which are given by $k_1 = k_{11} \otimes k_{12}$, where k_{11} and k_{12} are both single-qubit operations. To implement such a two-qubit local unitary k_1 , we need to implement both k_{11} and k_{12} within the same time. We can satisfy this constraint by making the oscillating control field that addresses one qubit to be resonant and that which addresses the other qubit to be slightly off resonance. Using this offset as an additional variable, we can then apply a numerical optimization procedure to achieve k_{11} and k_{12} simultaneously, leading to the desired local two-qubit unitary.

The above analysis of the time duration is made in the laboratory frame and thus differs from the standard NMR-ESR situation in which pulses are made in the rotating frame [18] [Eq. (17) applies only in the laboratory frame]. When working in the rotating frame $U_1 = e^{i\omega_0 t/2\sigma_z} U$, as is usual in NMR experiments at resonance, the following time constraints are instead required to implement U_T :

$$\phi - \pi/2 + 2m_1\pi = \delta, \quad (18)$$

$$\pi - \theta + 2m_2\pi = \frac{A}{2} t_f, \quad (19)$$

$$-\gamma + 2m_3\pi = \delta - \omega_0 t_z. \quad (20)$$

In this case, we have

$$t_f + t_z = \frac{2(\pi - \theta) + 4m_2\pi}{A} + \frac{\phi + \gamma - \pi/2 + 2m\pi}{\omega_0}.$$

Comparing Eqs. (14) and (18), we see that in the rotating frame there is no additional constraint on t_f , and therefore it is possible to decrease the time to reach a desired operation merely by increasing the amplitude of the oscillating field. This is not possible in the laboratory frame and thus the quantization of the time duration to implement a single-qubit operation in the laboratory frame is an intrinsic property for a general quantum mechanical system of the form of Eq. (6).

2. Nonperpendicular control field

We now consider the situation in which the control Hamiltonian is an oscillating electromagnetic field that is not perpendicular to the static field:

$$i\dot{U}_1 = \left[\frac{\omega_0}{2} \sigma_z + \frac{A}{2} \cos(\omega t + \delta) (\cos \zeta \sigma_z - \sin \zeta \sigma_x) \right] U_1. \quad (21)$$

Here the control Hamiltonian $H_c = \cos \zeta \sigma_z - \sin \zeta \sigma_x$, so the static and oscillating fields are tilted by an angle. This can arise in NMR or in coupled semiconductor quantum dots [19]. Let $U_2 = e^{i(\omega_0 t + \delta)/2\sigma_z} U_1$. Imposing the rotating-wave approximation again, we have

$$i\dot{U}_2 = \frac{A}{4} \{ 2 \cos \zeta \cos(\omega t + \delta) \sigma_z - \sin \zeta [\cos(\omega - \omega_0) t \sigma_x + \sin(\omega - \omega_0) t \sigma_y] \} U_2. \quad (22)$$

When the oscillating field ω is tuned at the resonant frequency ω_0 , Eq. (22) becomes

$$i\dot{U}_2 = \frac{A}{4} [2 \cos \zeta \cos(\omega_0 t + \delta) \sigma_z - \sin \zeta \sigma_x] U_2. \quad (23)$$

Letting $U_3 = e^{-i\pi/4\sigma_y} U_2$, we transform Eq. (23) into the standard form

$$i\dot{U}_3 = \frac{A}{4} [2 \cos \zeta \cos(\omega_0 t + \delta) \sigma_x + \sin \zeta \sigma_z] U_3. \quad (24)$$

Finally, letting $U_4 = e^{iA \sin \zeta/4\sigma_z} U_3$, we obtain

$$\begin{aligned} i\dot{U}_4 &= \frac{A}{2} \cos \zeta \cos(\omega_0 t + \delta) \left[\sigma_x \cos\left(\frac{A}{2} \sin \zeta t\right) - \sigma_y \sin\left(\frac{A}{2} \sin \zeta t\right) \right] U_4 \\ &= \frac{A}{4} \cos \zeta \left(\begin{array}{cc} 0 & e^{i[(\omega_0 - A/2 \sin \zeta)t + \delta]} + e^{i[-(\omega_0 - A/2 \sin \zeta)t - \delta]} \\ e^{i[(\omega_0 + A/2 \sin \zeta)t + \delta]} + e^{i[-(\omega_0 + A/2 \sin \zeta)t - \delta]} & 0 \end{array} \right) U_4. \end{aligned} \quad (25)$$

Since the control fields are usually high-frequency signals, we have $\omega_0 \gg A/2 \sin \zeta$. Equation (25) can then be simplified to

$$i\dot{U}_4 = \frac{A}{2} \cos \zeta \cos(\omega_0 t + \delta) \sigma_x U_4, \quad (26)$$

which has a solution

$$U_4(t) = e^{-iA \cos \zeta [\sin(\omega_0 t + \delta) - \sin \delta] / (2\omega_0) \sigma_x}. \quad (27)$$

Combining the above series of transformations, we obtain an approximate solution to Eq. (21) as

$$U(t_f) = e^{-i(\omega_0 t_f + \delta)/2 \sigma_z} e^{iA \sin \zeta / 4 \sigma_x t_f} \times e^{-i\{A \cos \zeta [\sin(\omega_0 t_f + \delta) - \sin \delta] / (2\omega_0) - \delta/2\} \sigma_z}. \quad (28)$$

As in the previous example, we also have the freedom to implement any arbitrary σ_z rotation by turning off the oscillating control field for a time duration t_z . Hence the final quantum operation achieved can be written as

$$\begin{aligned} U(t_f, t_z) &= U(t_f) e^{-i\omega_0/2 \sigma_z t_z} \\ &= e^{-i(\omega_0 t_f + \delta)/2 \sigma_z} e^{iA \sin \zeta / 4 \sigma_x t_f} \\ &\quad \times e^{-i\{A \cos \zeta [\sin(\omega_0 t_f + \delta) - \sin \delta] / (2\omega_0) - \delta/2 + \omega_0 t_z/2\} \sigma_z}. \end{aligned} \quad (29)$$

The time duration required to implement an arbitrary single-qubit operation under these conditions may be similarly derived by comparing with the general form of U_T given in Eq. (13). This results in the conditions

$$\phi - \pi/2 + 2m_1\pi = \omega_0 t_f + \delta, \quad (30)$$

$$\pi - \theta + 2m_2\pi = -\frac{A}{2} \sin \zeta t_f, \quad (31)$$

$$-\gamma + 2m_3\pi = -\frac{A \cos \zeta}{\omega_0} [\sin(\omega_0 t_f + \delta) - \sin \delta] + \delta - \omega_0 t_z, \quad (32)$$

where $m_1, m_2, m_3 \in \mathbb{Z}$ and $m_1 + m_2 + m_3$ is even. From Eqs. (30) and (32), we then find that

$$t_f + t_z = \left[\phi + \gamma - \frac{\pi}{2} + \frac{A \cos \zeta}{\omega_0} (\cos \phi + \sin \delta) + 2m\pi \right] / \omega_0, \quad (33)$$

where m is an integer. Thus when the oscillating control field is tuned at the resonant frequency, the total time to implement a single-qubit operation is also quantized in this case of an arbitrary nonperpendicular control field.

C. Piecewise constant control field

We now consider the case when the control v can be varied within a given range $[v_0, v_1]$. A well-known control strategy is bang-bang control, which pertains when the control field switches back and forth between two extremal values v_0 and v_1 [11]. In classical control theory, it can be

shown that bang-bang control is indeed the time-optimal control strategy for a double-integrator system. We will show that for a quantum system of the form in Eq. (2), bang-bang control can generate an arbitrary single-qubit operation with the minimum number of switchings. We note that the term bang-bang control has recently been adopted with a somewhat different meaning in the study of the dynamical coupling of open quantum systems [20–23], where it is referred to performing instantaneously, or as fast as physically possible, a set of unitaries, implying that the corresponding set of Hamiltonians can be turned on for negligible amounts of time with (ideally) arbitrarily large strength. A modified form of this approach for finite control field amplitudes and durations has been presented in Ref. [24].

We rewrite the quantum system (2) as follows:

$$i\dot{U} = (a\sigma_z + vH_c)U, \quad (34)$$

where $v \in [v_0, v_1]$. Without loss of generality, we can assume that $v_0 = 0$. By taking extremal values $v = 0$ and $v = v_1$, we obtain two linearly independent Hamiltonians

$$H_1 = a\sigma_z, \quad (35)$$

$$H_2 = a\sigma_z + v_1 H_c. \quad (36)$$

Our task is to achieve an arbitrary single-qubit target operation U_T by switching between H_1 and H_2 . The final operation generated by switching between these two Hamiltonians can be described as

$$U_T = e^{-iH_1 t_n} e^{-iH_2 t_{n-1}} \dots e^{-iH_1 t_3} e^{-iH_2 t_2} e^{-iH_1 t_1}. \quad (37)$$

In the mathematical literature, this problem is also known as the uniform finite-generation problem on Lie groups and can be traced back to the early 1970s [25,26]. Recently, D'Alessandro studied the optimal evaluation of generalized Euler angles on the rotation group with this approach [27].

To solve this problem, we first rewrite H_2 as

$$H_2 = a\sigma_z + v_1 H_c = b_1 \sigma_x + b_2 \sigma_y + b_3 \sigma_z.$$

Let $k = e^{i\sigma_z \gamma}$, where γ satisfies

$$-b_1 \sin 2\gamma + b_2 \cos 2\gamma = 0. \quad (38)$$

From the Campbell-Baker-Hausdorff (CBH) formula [28], we have

$$\tilde{H}_1 = k a \sigma_z k^\dagger = a \sigma_z,$$

$$\begin{aligned} \tilde{H}_2 &= k H_2 k^\dagger = e^{i\sigma_z \gamma} (b_1 \sigma_x + b_2 \sigma_y + b_3 \sigma_z) e^{-i\sigma_z \gamma} \\ &= (b_1 \cos 2\gamma + b_2 \sin 2\gamma) \sigma_x + b_3 \sigma_z \\ &= b(\sin \alpha \sigma_z + \cos \alpha \sigma_x), \end{aligned} \quad (39)$$

where

$$b = \sqrt{(b_1 \cos 2\gamma + b_2 \sin 2\gamma)^2 + b_3^2} \quad (40)$$

and

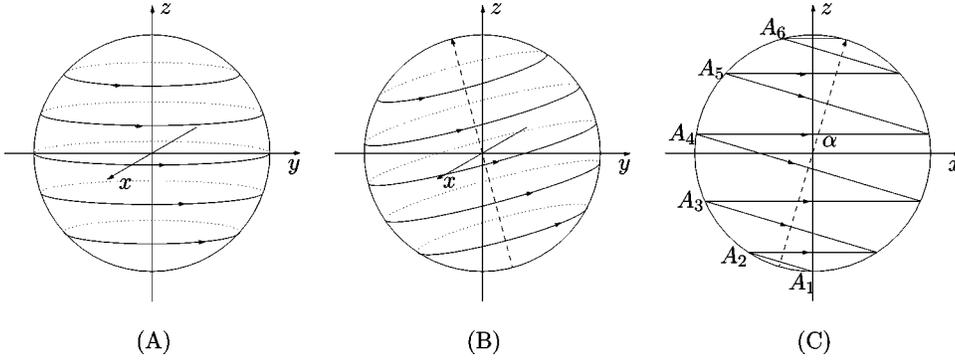


FIG. 3. Effect of the rotations $e^{-iH_1 t}$ (A) and $e^{-iH_2 t}$ (B) on the state of a single qubit. (A) A rotation about the z axis, (B) a rotation about the axis $\hat{n} = (\cos(\pi/6), 0, \sin(\pi/6))$, and (C) successive switching between the two rotations (A) and (B) applied with finite time durations allows any point on the Bloch sphere to be reached.

$$\begin{aligned} \sin \alpha &= \frac{\langle \tilde{H}_1, \tilde{H}_2 \rangle}{\langle \tilde{H}_1, \tilde{H}_1 \rangle^{1/2} \langle \tilde{H}_2, \tilde{H}_2 \rangle^{1/2}} = \frac{\text{tr}(\tilde{H}_1 \tilde{H}_2)}{\text{tr}(\tilde{H}_1^2)^{1/2} \text{tr}(\tilde{H}_2^2)^{1/2}} \\ &= \frac{\text{tr}(H_1 H_2)}{\text{tr}(H_1^2)^{1/2} \text{tr}(H_2^2)^{1/2}}. \end{aligned} \quad (41)$$

Without loss of generality, we can take $\alpha \in [-\pi/2, \pi/2]$. When the target operation U_T can be generated in bang-bang strategy as in Eq. (37), we have

$$\begin{aligned} kU_T k^\dagger &= k e^{-iH_1 t_n} e^{-iH_2 t_{n-1}} \dots e^{-iH_1 t_3} e^{-iH_2 t_2} e^{-iH_1 t_1} k^\dagger \\ &= e^{i\tilde{H}_1 t_n} e^{i\tilde{H}_2 t_{n-1}} \dots e^{i\tilde{H}_1 t_3} e^{i\tilde{H}_2 t_2} e^{i\tilde{H}_1 t_1}. \end{aligned}$$

In order to generate the target quantum operation U_T from the original quantum system (34), we therefore only need to generate $kU_T k^\dagger$ from the two Hamiltonians \tilde{H}_1 and \tilde{H}_2 in Eq. (39). For the special case $\alpha=0$, we have $\tilde{H}_2 = b\sigma_x$ and U_T simplifies to the familiar Euler ZZZ decomposition of Eq. (13):

$$U_T = e^{-i(\phi-\pi/2)/2\sigma_z} e^{-i(\pi-\theta)/2\sigma_x} e^{-i\gamma/2\sigma_z}.$$

The Bloch sphere steering technique can now be used to find the time sequences for switching between H_1 and H_2 . We know that the effect of $e^{-iH_1 t}$ on the quantum state $|1\rangle$ is a rotation about the z axis, whereas the effect of $e^{-iH_2 t}$ is a rotation about the axis $(\sin \alpha, 0, \cos \alpha)$, as shown in Figs. 3(A) and 3(B). Application of the time sequence given in Eq. (37) to the quantum state $|1\rangle$ results in an alternation of rotations about these two axes, illustrated in Fig. 3(C). Therefore, to generate U_T , we need to reach the point $U_T|1\rangle$ from the south pole $|1\rangle$ on the Bloch sphere by switching back and forth between two rotations. It is evident that we can now achieve any arbitrary point on the Bloch sphere, by using these two rotations in alternation, with finite switching times. The solution for the number of switches and time durations is illustrated explicitly by the following example.

1. Example: Bang-bang solution for the Hadamard gate

Suppose that in the single-qubit system (2), we have $v \in [0, a\sqrt{3}]$. This gives the following two Hamiltonians defined by the extremal values of v :

$$H_1 = a\sigma_z,$$

$$H_2 = 2a \left(\sin \frac{\pi}{6} \sigma_z + \cos \frac{\pi}{6} \sigma_x \right). \quad (42)$$

We aim to generate the Hadamard gate

$$U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

by switching between these two finite Hamiltonians at well-defined times. We first find the point corresponding to the Hadamard gate U_H on the Bloch sphere. Computing

$$\Phi(U_H) = U_H|1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and using Eq. (5), we find that U_H corresponds to the point $(\theta, \phi) = (\pi/2, \pi)$ on the Bloch sphere. The Hamiltonians H_1 and H_2 of Eq. (42) generate two rotations on the Bloch sphere: one about the z axis and the other about the axis $\hat{n} = (\cos(\pi/6), 0, \sin(\pi/6))$ (see Fig. 4). We can implement the Hadamard gate U_H by switching between these two rotations as follows:

$$U_H = -i e^{-iH_1 t_3} e^{-iH_2 t_2} e^{-iH_1 t_1},$$

where $t_1 = 9.90/a$ and $t_2 = t_3 = (1/2a)\cos^{-1}(1/\sqrt{3})$. From Fig. 4, it is also clear that for this Hamiltonian, we can generate any arbitrary single-qubit operation with at most three switchings.

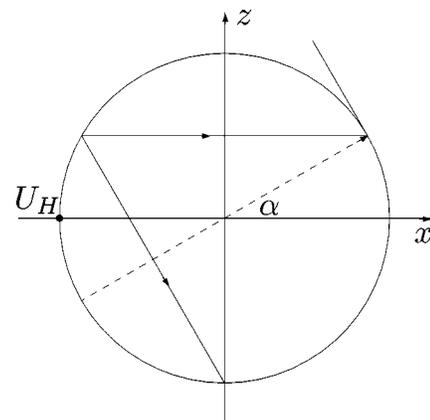


FIG. 4. Two rotations generated by the Hamiltonians given in Eq. (42).

The minimum number of switchings between the two Hamiltonians H_1 and H_2 needed to generate a target quantum operation U_T is determined by the rotation axis $(\sin \alpha, 0, \cos \alpha)$ and the z coordinate of the point $U_T|1\rangle$ on the Bloch sphere. When $\alpha=0$, we can get to any point on the sphere starting from the south pole ($|1\rangle$) by at most two switchings. This corresponds to the Euler ZZZ decomposition. For a general value of $\alpha \in [0, \pi/2]$, it is not hard to derive that the coordinates for A_n in Fig. 3(C) are $A_n = [\cos \alpha_n, -\sin \alpha_n]$, where $\alpha_n = \pi/2 + 2(n-1)(\pi/2 - \alpha)$. To ensure that any point on the sphere can be reached by the combination of these two rotations, we only require the condition that $\alpha_n \geq 3\pi/2$, which in turn yields that we can implement any arbitrary single-qubit operation with at most $\lceil \pi/(\pi/2 - \alpha) \rceil$ switchings, where the ceiling function $\lceil x \rceil$ is defined as a function that rounds x to the nearest integer towards infinity. Similarly, when $\alpha \in (\pi/2, \pi]$, the maximal switchings needed are $\lceil \pi/(\alpha - \pi/2) \rceil$. To achieve the minimum number of switchings, we therefore need to use the extremal values of the control to minimize the angle α .

We note that the generation of arbitrary single-qubit operations by switching between two constant control fields has many other applications in quantum computation and quantum information processing. For example, in quantum simulations, if we are given two single-qubit Hamiltonians H_1 and H_2 , the usual way to generate $U = e^{iH\Delta t}$ is to use the Trotter formula [29–31]

$$e^{i(H_1+H_2)\Delta t} = e^{iH_1\Delta t}e^{iH_2\Delta t} + O(\Delta t^2).$$

We can use the above bang-bang approach to simulate $U = e^{iH\Delta t}$ in a constructive and exact manner, without the assumption of impulsive and arbitrarily strong controls [20] or of infinitesimal operations [32]. Another example is in encoded universal quantum computation with the exchange interaction [33]. Here the encoded single-qubit quantum gates are generated by two Hamiltonians identical to those in Eq. (42). The switching sequence to implement any such encoded single-qubit operation can readily be derived using the strategy outlined above, which yields the result that only four switches are necessary, corresponding to the solution found by numerical arguments in [33]. Finally, it has been shown recently that electron spin in a semiconductor heterostructure may be controlled by a single-qubit Hamiltonian generated by g -tensor engineering that is realized by applying a dc bias voltage [34]. The present analysis shows that by switching between two Hamiltonians obtained from two different g factors corresponding to different bias voltages, one can thus implement any single-qubit quantum operation.

III. GENERATION OF TWO-QUBIT OPERATIONS: STEERING IN THE WEYL CHAMBER

To generate an arbitrary quantum operation on arbitrarily many qubits, the target quantum operation can be decomposed into a combination of single- and two-qubit operations [1]. In this section we now consider the generation of two-qubit operations.

A general Hamiltonian for a two-qubit quantum physical system can be written as

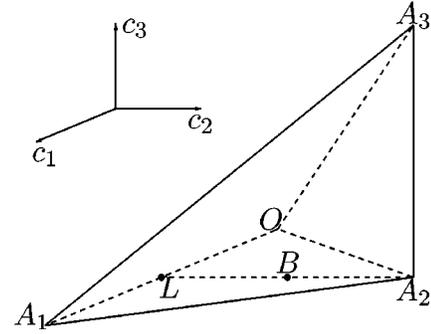


FIG. 5. Tetrahedral (or Weyl chamber) representation of local equivalence classes of nonlocal two-qubit operations from Ref. [15]. Points within the tetrahedron are labeled $[c_1, c_2, c_3]$, where $\pi - c_2 \geq c_1 \geq c_2 \geq c_3 \geq 0$. Points $O([0, 0, 0])$ and $A_1([\pi, 0, 0])$ correspond to local operations, $L([\pi/2, 0, 0])$ to the CNOT gate, and $A_3([\pi/2, \pi/2, \pi/2])$ to the SWAP gate.

$$H = g_1 \cdot \vec{\sigma} \otimes I + I \otimes g_2 \cdot \vec{\sigma} + S, \quad (43)$$

where $\vec{\sigma}$ is the vector $(\sigma_x, \sigma_y, \sigma_z)$ of Pauli matrices and $S = \sum J_{\alpha\beta} \sigma_\alpha^1 \sigma_\beta^2$ with $\sigma_\alpha^1 \sigma_\beta^2 = \sigma_\alpha \otimes \sigma_\beta$, $\alpha, \beta \in \{x, y, z\}$, and $J_{\alpha\beta}$ the corresponding coupling strength. The coefficients $g_1 = [g_{1x}, g_{1y}, g_{1z}]$ and $g_2 = [g_{2x}, g_{2y}, g_{2z}]$ may be regarded as single-qubit “ g factors,” although they may have very different physical origins, depending on the physical realization of the qubits. From [10,15,29], we know that for any arbitrary set of coupling strengths $\{J_{\alpha\beta}\}$, there exists a local operation k such that

$$kSk^\dagger = J_x \sigma_x^1 \sigma_x^2 + J_y \sigma_y^1 \sigma_y^2 + J_z \sigma_z^1 \sigma_z^2. \quad (44)$$

Without loss of generality, we can assume for the two-qubit steering problem that the two-body interaction term S is always given as in Eq. (44). We shall study the generation of an arbitrary quantum operation from relevant physical Hamiltonians by a tuning of the parameters g_1, g_2 and J_x, J_y, J_z , all of which correspond to control parameters, in this context.

In Ref. [15] we have shown that this problem can be reduced to a steering problem in a tetrahedron. Central to this analysis is the notion of local equivalence. Two quantum operations $U, U_1 \in \text{SU}(4)$ are called locally equivalent if they differ only by local operations: $U = k_1 U_1 k_2$, where $k_1, k_2 \in \text{SU}(2) \otimes \text{SU}(2)$ are both local operations. Clearly this defines an equivalence relation on the Lie group $\text{SU}(4)$ of all two-qubit operations. It was shown in [15] that the local-equivalence classes of two-qubit operations are in one-to-one correspondence with the points in the tetrahedron $OA_1A_2A_3$ as shown in Fig. 5, except on its base (where there is a one-to-two correspondence). This tetrahedron is a Weyl chamber that contains all possible local-equivalence classes. To locate the point in the tetrahedron that corresponds to a given two-qubit operation, we make use of a set of local invariants. Reference [14] provides a simple procedure to compute three real quantities g_1, g_2 , and g_3 for a given two-qubit operation and showed that two quantum operations are locally equivalent if and only if they have identical values of

these three invariants. These local invariants can be expressed in terms of the tetrahedron coordinates $[c_1, c_2, c_3]$ as follows [15]:

$$\begin{aligned} g_1 &= 4 \cos c_1 \cos c_2 \cos c_3, \\ g_2 &= 4 \sin c_1 \sin c_2 \sin c_3, \\ g_3 &= \cos 2c_1 + \cos 2c_2 + \cos 2c_3. \end{aligned} \quad (45)$$

By solving Eqs. (45), we can obtain the point $[c_1, c_2, c_3]$ in the tetrahedron that represents a given two-qubit operation.

As time evolves, the quantum system controlled by H generates a continuous flow in the space of all quantum operations. At any time instant t , the quantum operation $U(t)$ on this flow can be mapped to a point in the tetrahedron. This defines a continuous trajectory within the Weyl chamber. We then employ a two-step procedure to generate a target two-qubit operation from a given Hamiltonian. First, we steer the Weyl chamber trajectory generated by the given Hamiltonian H to reach the point representing the local-equivalence class of the desired target operation. Second, we perform the necessary local operations that transform the quantum operation at this Weyl chamber point to the true target operation. The single-qubit operations are generated as described in Sec. II. Therefore we only deal with the first step here: namely, steering of the system Hamiltonian H to generate a trajectory that hits the target in the tetrahedron $OA_1A_2A_3$.

For a general Hamiltonian containing both local and nonlocal terms, it is usually difficult to implement an arbitrary two-qubit operation directly. This is reflected in the complexity of a general trajectory in the Weyl chamber. One approach is to introduce an intermediate step to construct a universal gate set of elementary gates that can be used to construct any arbitrary two-qubit operation [1]. An alternative perspective is to seek to minimize the time for nonlocal operations [10,35]. We follow the first approach of steering to achieve a universal gate here. The solutions will then not necessarily be time optimal. Optimization for time can be performed subsequently in comparison of different gates [36].

One well-known example of such a universal gate set is the CNOT gate together with single-qubit operations [1]. In [37], we showed that both CNOT and double-CNOT (or its locally equivalent variant iSWAP [38,39]) operations require at most three applications to realize any two-qubit operation. More recently, we discovered a new quantum operation B that is universal by at most two applications together with at most six single-qubit operations [36]. Whenever the direct generation of any quantum operation is difficult, we can take advantage of these results for efficient two-qubit quantum circuits and first seek to implement the quantum gate B or CNOT, then use the corresponding analytic circuits of [36,37] in order to construct an arbitrary two-qubit operation.

To illustrate the basic idea of the steering approach, consider first a simple case when $g_1 = g_2 = 0$; i.e., the Hamiltonian contains only the nonlocal term S . The Weyl chamber trajectory generated by this Hamiltonian is the straight line $U(t) = [J_x, J_y, J_z]t$ [15]. The evolution direction of this line can be

changed by conjugating with an appropriate local operation from the Weyl group. Since the tetrahedron is a three-dimensional geometric object, it is evident that by changing the direction at most twice, we can steer the Hamiltonian to anywhere in the tetrahedron. In other words, by turning on the Hamiltonian at most three times, together with application of at most four local gates, we can implement any arbitrary two-qubit operation [15]. Note that when the local terms commute with the nonlocal term, we can drop the local terms and the trajectory is unchanged. For example, with $H = g_{1x}\sigma_x^1 + g_{2x}\sigma_x^2 + J_x\sigma_x^1\sigma_x^2$, corresponding to the Hamiltonian derived in the superconducting qubit proposal of [40], the Weyl chamber trajectory is exactly the same as that generated by $J_x\sigma_x^1\sigma_x^2$ —namely, along the straight line OA_1 . In this case, the straight line trajectory leads directly from the origin (local unitary) to the CNOT gate $[\pi/2, 0, 0]$. This result was derived by more complex means in Ref. [40].

A. Isotropic qubit coupling

Isotropic coupling of qubits, characterized by coupling amplitudes $J_x = J_y = J_z = J$, is a very common form of two-body interaction that appears in many physical qubit proposals involving electronic spins—e.g., spin-coupled quantum dots [41,42] and donor spins in semiconductors [43–47]. We present here two different strategies to steer the Weyl chamber trajectories generated by this Hamiltonian, both of which are based on the ability to tune the relative values of the single-qubit parameters g_1 and g_2 . The technological ability to make this tuning has been demonstrated for electron spins in semiconductors in Ref. [34]. For greater simplicity, in the remainder of this section we use a slightly modified notation for the two-qubit interaction: namely, the form JS where $S = \sigma_x^1\sigma_x^2 + \sigma_y^1\sigma_y^2 + \sigma_z^1\sigma_z^2$ and J is the isotropic coupling amplitude.

The first strategy is based on tuning g_1 and g_2 to be equal—i.e., setting $g_1 = g_2$. Then the individual components of the total single-qubit spins commute with the interaction term S ,

$$[\sigma_x^1 + \sigma_x^2, S] = 0, \quad [\sigma_y^1 + \sigma_y^2, S] = 0, \quad [\sigma_z^1 + \sigma_z^2, S] = 0.$$

This implies that single-qubit and two-qubit terms commute,

$$\begin{aligned} [g_1 \cdot \vec{\sigma} \otimes I + I \otimes g_1 \cdot \vec{\sigma}, S] &= [g_{1x}(\sigma_x^1 + \sigma_x^2) + g_{1y}(\sigma_y^1 + \sigma_y^2) \\ &\quad + g_{1z}(\sigma_z^1 + \sigma_z^2), S] = 0, \end{aligned}$$

allowing the time evolution to be factorized exactly:

$$e^{iHt} = e^{ig_1 \cdot \vec{\sigma} t} \otimes e^{ig_2 \cdot \vec{\sigma} t} e^{iJS t}.$$

Consequently, the flow generated by the Hamiltonian H in the tetrahedron is the same as that generated by S ; i.e., we have achieved a reduction to the purely nonlocal interaction. The resulting Weyl chamber trajectory lies along the line OA_3A_1 , and we can achieve the CNOT gate by changing the evolution direction just once (cf. example 4 in Ref. [15]). We emphasize that this reduction results from the tuning of the two single-qubit terms to achieve commutation with the interaction term. Furthermore, it is valid independent of the nature of the single-qubit terms—i.e., whether they involve

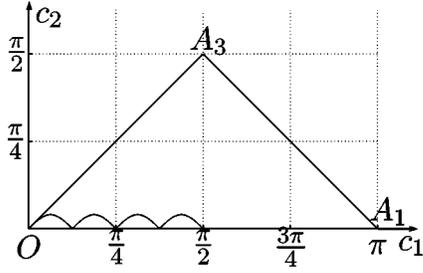


FIG. 6. Weyl chamber trajectory obtained upon steering the isotropic Hamiltonian to reach the CNOT gate by tuning the local terms g_1 and g_2 to be linearly dependent. The Weyl chamber trajectory is located in the OA_3A_1 plane of the tetrahedron and goes from the origin to the point $[\pi/2, 0, 0]$ representing the local equivalence class of CNOT operations, with a total of four oscillations.

σ_x , σ_y , and/or σ_z . Thus, although the result resembles the known result that the isotropic exchange interaction generates a $\sqrt{\text{SWAP}}$ gate from which a CNOT gate can be obtained by conjugating with single-qubit gates [48], it is valid here for a more general Hamiltonian that contains both nonlocal and local terms. The extended range of validity is a consequence of the decomposition of the two-qubit operation into nonlocal-equivalence classes and local operations.

The second strategy is based on tuning the single-qubit parameters g_1 and g_2 such that they become linearly dependent—i.e., $g_1 = \lambda g_2$, where λ describes the parameter ratio. This is clearly a less stringent tuning requirement than the first strategy. After some mathematical analysis, the trajectory generated by the Hamiltonian in the tetrahedron is found to be

$$c_1 = 2Jt,$$

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

where $\omega = \sqrt{(\lambda - 1)^2 \|g_2\|^2 + 4J^2}$. Since $c_2 = c_3$, the entire trajectory lies in the OA_3A_1 plane of the tetrahedron $OA_1A_2A_3$, as shown in Fig. 6. The CNOT gate is located on the intersection of this plane with the base of the tetrahedron, at $[\pi/2, 0, 0]$, and hence constitutes a natural target for these trajectories. It is readily verified that in order to steer the trajectory to the CNOT gate we only need to satisfy the conditions

$$2Jt = \frac{\pi}{2}, \quad (46)$$

$$\omega t = m\pi, \quad (47)$$

where m is a positive integer. From these two equations, we find that the time required to reach the CNOT gate with this trajectory is $t = \pi/4J$, and the parameter ratio λ has to satisfy the condition

$$(\lambda - 1)^2 \|g_2\|^2 = (16m^2 - 4)J^2. \quad (48)$$

From Eq. (46), we find that the time to achieve the CNOT gate depends only on the coupling strength J , while Eq. (47) shows that the integer m determines the number of oscillations in the trajectory.

It is interesting to note that this time is equal to the time needed to achieve the CNOT gate from a purely isotropic Hamiltonian JS or from the first strategy discussed above, both of which have a straight line Weyl chamber trajectory [15].

As an example, consider a system with $J=0.1$ and choose $m=4$. Then Eq. (48) becomes

$$(\lambda - 1)^2 \|g_2\|^2 = 2.52,$$

which needs to be solved for λ , given a specific set of g parameters. Choosing $g_2 = [4, 4, 4]$, we obtain $\lambda = 0.7709$, $\omega = 1.6$, and find a time $t = 2.5\pi$ to reach the CNOT gate. The resulting Weyl chamber trajectory is shown in Fig. 6.

B. Anisotropic qubit coupling

Hamiltonians of the general form of Eq. (43) with anisotropic coupling coefficients $J_{\alpha\beta}$ are encountered in many proposed solid-state implementations of quantum computation. These include quantum dots [49], electrons coupled by long-range quantum Hall effects [50], electrons on helium [51], and atoms in cavities [52].

To illustrate the Weyl chamber steering approach for anisotropic qubit couplings, we consider here a Hamiltonian containing an Ising interaction—i.e., a single diagonal component of $J_{\alpha\beta}$ only:

$$H_{yy} = g_{1x}\sigma_x^1 + g_{1z}\sigma_z^1 + g_{2x}\sigma_x^2 + g_{2z}\sigma_z^2 + J\sigma_x^1\sigma_x^2.$$

This Ising-type coupling between qubits is commonly seen in proposals for superconducting Josephson junction qubits [12,53] and also arises as one limit of dipole-dipole or J -coupling systems [18,54]. It is straightforward to show that the Hamiltonian H_{yy} is locally equivalent to the corresponding Hamiltonians H_{xx} and H_{zz} :

$$H_{xx} = g_{1y}\sigma_y^1 + g_{1z}\sigma_z^1 + g_{2y}\sigma_y^2 + g_{2z}\sigma_z^2 + J\sigma_x^1\sigma_x^2,$$

$$H_{zz} = g_{1x}\sigma_x^1 + g_{1y}\sigma_y^1 + g_{2x}\sigma_x^2 + g_{2y}\sigma_y^2 + J\sigma_z^1\sigma_z^2.$$

Consequently the Weyl chamber trajectories generated by H_{xx} and H_{zz} are the same as those generated by H_{yy} . Using Makhlin's procedure [14] to evaluate the local invariants of $U(t) = e^{iH_{yy}t}$, we find

$$g_1 = \frac{(f_1^2 + J^2)J^2x^2 + (f_2^2 + J^2)J^2y^2 + f_1^2f_2^2 - J^4}{(f_1^2 + J^2)(f_2^2 + J^2)},$$

$$g_2 = 0,$$

$$g_3 = [3f_1^2f_2^2 - J^2(f_1^2 + f_2^2) + J^4(8x^2y^2 + 3) + 4J^2y^2(f_2^2 - J^2) + 4J^2x^2(f_1^2 - J^2)] / (f_1^2 + J^2)(f_2^2 + J^2), \quad (49)$$

where $x = \cos \sqrt{f_2^2 + J^2}t$, $y = \cos \sqrt{f_1^2 + J^2}t$, $f_1 = \sqrt{g_{1x}^2 + g_{1z}^2 + \sqrt{g_{2x}^2 + g_{2z}^2}}$, and $f_2 = \sqrt{g_{1x}^2 + g_{1z}^2} - \sqrt{g_{2x}^2 + g_{2z}^2}$. Without loss of generality, we can assume that $J=1$ in the subsequent analysis.

It turns out that both CNOT and B gates can be generated by turning on this anisotropic Hamiltonian only once. The B gate is more efficient than the CNOT gate in representing

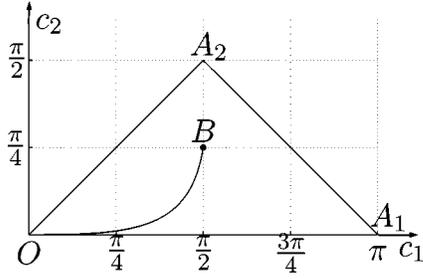


FIG. 7. Minimum-time Weyl chamber trajectory that reaches the B gate from the Ising-type YY interaction in one switching. See Fig. 5 for definitions of the coordinates and special points.

arbitrary two-qubit operations [36] and may therefore be more useful for quantum simulations, while the CNOT gate is required for many common error correction protocols. We first consider realization of the B gate. The local invariants are $g_1=g_2=g_3=0$ [36]. To find the Weyl chamber trajectory that reaches the point $B=[\pi/2, \pi/4, 0]$ in time t we need therefore only to set $g_1=g_3=0$ in Eq. (49). This yields the following equations for t that must be satisfied simultaneously:

$$\cos(2\sqrt{f_1^2+1}t) = -f_1^2 \pm \frac{\sqrt{2}}{2}(f_1^2+1),$$

$$\cos(2\sqrt{f_2^2+1}t) = -f_2^2 \mp \frac{\sqrt{2}}{2}(f_2^2+1).$$

There are infinitely many solutions to these two equations, depending on the combination of single-qubit parameters $g_{i\alpha}$. Numerical analysis reveals that the time-optimal solution for reaching the B gate is achieved by setting $f_1=1.6753$, $f_2=0$, with terminal time $t=3\pi/8$. The corresponding Weyl chamber trajectory is shown in Fig. 7. Note that this time-optimal trajectory remains at all times in the basal plane of the tetrahedron $OA_1A_2A_3$. A similar analysis was made in [15] for a particular instance having $g_{1x}=g_{2x}=-\alpha/2$, $g_{1z}=g_{2z}=0$, and $J=\alpha^2$.

We next consider realization of the CNOT gate. The local invariants for the CNOT gate are $g_1=g_2=0$ and $g_3=1$ [14]. Solving Eq. (49) we obtain the following two equations:

$$\cos 2\sqrt{f_1^2+1}t = -f_1^2,$$

$$\cos 2\sqrt{f_2^2+1}t = -f_2^2.$$

By numerical analysis, we find that the minimum time to achieve the CNOT gate is $t=3.2551$, with $f_1=0.9516$ and $f_2=0.9492$. Comparing this with the time-optimal solution for reaching the B gate described above, it is clear that for such an Ising-type coupling, the B gate can be generated in shorter time than the CNOT gate.

C. Weak qubit coupling

In many coupled qubit systems, the two-qubit interaction term is much weaker than the local term; that is, J is small in

comparison to g_1 and g_2 . For example, this is the case in circuits of flux qubits coupled by a mutual inductance that is controlled by the circulating current in a dc superconducting quantum interference device (SQUID) [19]. It is also the case in most NMR systems of exchange-coupled nuclear spins [18]. Estimates of parameters for exchange-coupled electron spins in quantum dots also put these systems in this weak-coupling regime at magnetic field strengths relevant to experiments [42,55–57]. In such situations we have found that the Weyl chamber trajectory can be approximated to good accuracy by some simple curves within the tetrahedron. This provides a useful strategy in many physical systems, where instead of attempting to control the exact time evolution, we seek rather to steer only the approximating curves in the Weyl chamber and may wish to incorporate additional factors into numerical optimization protocols.

We first consider a simple case: namely, tuning g_1 and g_2 such that their norms are equal—i.e., $\|g_1\|=\|g_2\|$. In this case, when in addition $J \ll \|g_i\|$, the trajectory generated in the tetrahedron can be well approximated by a straight line. Specifically, when the Hamiltonian is given in the Ising form

$$H = g_1 \cdot \vec{\sigma} \otimes I + I \otimes g_2 \cdot \vec{\sigma} + J_z \sigma_z^1 \sigma_z^2,$$

with $\|g_1\|=\|g_2\|$ and J_z small, the resulting Weyl chamber trajectory can be approximated by the following straight lines:

$$[c_1, c_2, c_3] = \begin{cases} \frac{J_z t}{\|g_1\|^2} [2g_{1z}g_{2z}, \rho, \rho], & \text{if } 2g_{1z}g_{2z} \geq \rho, \\ \frac{J_z t}{\|g_1\|^2} [\rho, \rho, 2g_{1z}g_{2z}], & \text{if } 2g_{1z}g_{2z} < \rho, \end{cases}$$

where $\rho = \sqrt{g_{1x}^2 + g_{1y}^2} \sqrt{g_{2x}^2 + g_{2y}^2}$. Recall that in the case when the Hamiltonian is purely nonlocal—i.e., it contains no single-qubit terms—the Weyl chamber trajectory is a straight line and we can generate any arbitrary two-qubit operation by applying local unitaries to change the evolution direction of the trajectory. We can use the same technique here to steer the Weyl chamber trajectory to arrive at any point in the tetrahedron with at most two switchings.

For the general case when $\|g_1\| \neq \|g_2\|$ and $S = J_x \sigma_x^1 \sigma_x^2 + J_y \sigma_y^1 \sigma_y^2 + J_z \sigma_z^1 \sigma_z^2$, we find that the trajectory can be well approximated by the following sinusoidal curve in the tetrahedron:

$$c_1 = \frac{J_x g_{1x} g_{2x} + J_y g_{1y} g_{2y} + J_z g_{1z} g_{2z}}{\|g_1\| \|g_2\|} 2t,$$

$$c_2 = c_3 = p(g_1, g_2) |\sin(\|g_1\| - \|g_2\|)t|, \quad (50)$$

where p is a nonzero function of g_1 and g_2 . From Eq. (50), the approximate curve stays in the plane OA_3A_1 and moves away from the origin in the direction of the CNOT gate. Therefore, for this Hamiltonian, the CNOT gate is a natural choice of target operation. To reach the CNOT gate, we require that Eq. (50) be satisfied with values $c_1=\pi/2$ and $c_2=c_3=0$. It is clear that the form of the function p is irrelevant. Consequently, we need only to satisfy the following two equations:

$$\frac{J_x g_{1x} g_{2x} + J_y g_{1y} g_{2y} + J_z g_{1z} g_{2z}}{\|g_1\| \|g_2\|} 2t = \frac{\pi}{2},$$

$$(\|g_1\| - \|g_2\|)t = m\pi, \quad (51)$$

where m is an integer. To illustrate this approach, consider the following example of weak coupling:

$$H = g_1 \cdot \vec{\sigma} \otimes I + I \otimes g_2 \cdot \vec{\sigma} + 0.2\sigma_z^1 \sigma_z^2. \quad (52)$$

Here the local terms g_1 and g_2 are one order larger than the interaction strength $J_z=0.2$. From Eq. (51), we find that the local terms g_1 and g_2 must satisfy

$$\frac{0.2g_{1z}g_{2z}}{\|g_1\| \|g_2\| (\|g_1\| - \|g_2\|)} = \frac{1}{4m}. \quad (53)$$

Setting, e.g., $m=3$, we derive one solution for Eq. (53) as $g_1=[2.5, 0, 10.0182]$ and $g_2=[2, 0, 7.8177]$. After a time duration $t=4.1778$, this Hamiltonian can achieve a gate located at $[0.5000, 0.0002, 0.0002]\pi$, which is very close to the CNOT gate. The Weyl chamber trajectory is shown in Fig. 8, where the solid line is the real trajectory generated by the Hamiltonian and the dotted line is the approximate sinusoidal curve. A realistic application of this example was recently made in Ref. [19] to inductively coupled flux qubits for which $\|g_1\| \neq \|g_2\|$ and $J_x=J_y=0$.

IV. CONCLUSIONS

We have developed a systematic approach to generate arbitrary two-qubit quantum operations by steering the unitary evolution corresponding to local and nonlocal interactions. The generation of single-qubit quantum gates was shown to

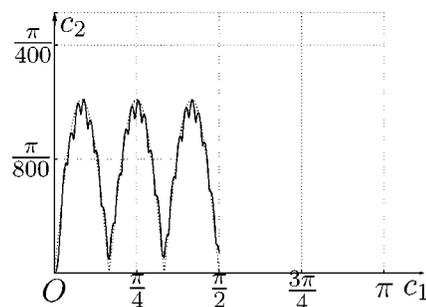


FIG. 8. Weyl chamber trajectory designed to reach the CNOT gate and generated by the weak two-qubit interaction given in Eq. (52). The trajectory is at all times in or very close to the OA_3A_1 plane of the tetrahedron $OA_1A_2A_3$ of Fig. 5.

map onto a steering problem on the Bloch sphere. Local two-qubit gates corresponding to coupled single-qubit gates can then be generated by combined steering on two coupled Bloch spheres. The nonlocal components of two-qubit gates were shown to be analyzable as a steering problem in a Weyl chamber of local equivalence classes. We applied this steering approach here to the generation of two-qubit quantum gates in several physical examples relevant to solid-state implementations of quantum information processing. The methods described here are expected to provide useful guidance to experimental design of circuits and pulse sequences for realization of quantum logic gates.

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