Exact Two-Qubit Universal Quantum Circuit

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We provide an analytic way to implement any arbitrary two-qubit unitary operation, given an entangling two-qubit gate together with local gates. This is shown to provide explicit construction of a universal quantum circuit that exactly simulates arbitrary two-qubit operations in SU(4). Each block in this circuit is given in a closed form solution. We also provide a uniform upper bound of the applications of the given entangling gates, and find that exactly half of all the controlled-unitary gates satisfy the same upper bound as the CNOT gate. These results allow for the efficient implementation of operations in SU(4) required for both quantum computation and quantum simulation.

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Construction of explicit quantum circuits that are universal, i.e., can implement any arbitrary unitary operation, plays a central role in physical implementations of quantum computation and quantum information processing [1,2]. Despite considerable efforts, there are still very few examples of exact universal quantum circuits. Most universality results are not constructive, following instead the approximative paradigm outlined by Lloyd [3] and Deutsch *et al.* [4], who showed that almost any quantum gate for two or more qubits can approximate any desired unitary transformation to arbitrary accuracy. Specific results of Barenco *et al.* [5] showing that a combination of quantum controlled-NOT (CNOT) and single-qubit gates is universal in the sense that any unitary operation on arbitrarily many qubits can be exactly expressed as a composition of these gates have led to the commonly adopted paradigm (''standard model'') of CNOT and single-qubit rotations. Brylinski and Brylinski [6] showed more generally that a two-qubit gate can provide universality with local gates if and only if it is entangling. However, this proof is not constructive and does not provide exact gate sequences for general operations, whereas in practical applications it is essential to find a *constructive* way to realize the two-qubit gates from a given entangling gate and local gates. Bremner *et al.* [7] have recently developed a constructive approach to implement the CNOT gate that relies on numerical procedures.

We have previously constructed a quantum circuit that contains at most three nonlocal gates generated by a given pure two-body Hamiltonian for finite time durations, supplemented with at most four local gates [8]. Using a geometric theory, we proved that such a quantum circuit can simulate any arbitrary two-qubit operation exactly and is therefore universal. However, in many physical applications, one may have little flexibility in choice of Hamiltonian or time duration. In this situation, what we can access is often a prescribed entangling gate U_g which is generated by a Hamiltonian over a fixed time duration. We present here an exact analytical approach to construct exact universal quantum circuits from such an arbitrary given entangling gate together with local gates. Our approach is based on the recognition in [6] that, given the group of two-qubit gates with subgroup H of local gates, $H' = U_g H U_g^{-1}$ is also a subgroup, where U_g is a given entangling gate. It can then be shown that the Lie algebras of H and H' generate su(4), the Lie algebra of the special unitary group SU(4). We develop an analytic realization of H' and use this to construct an exact quantum circuit for any arbitrary two-qubit operation in SU(4). Each step in the construction of the quantum circuit is given in a closed form solution.

One of the main features of this work is that we provide a uniform upper bound of the applications of the given entangling gate U_g; i.e., regardless of which two-qubit operation is to be implemented, we can always construct an exact quantum circuit in which the applications of the given entangling gate do not exceed the prescribed number. Existence of a uniform upper bound with a relatively small number for any given entangling gate provides an important estimation of overhead for experimentalists considering different physical implementations of two-qubit operations. The value of this upper bound depends solely on the nonlocal part of the given entangling gate. Specifically, we find that at most six applications of the CNOT gate suffice to implement any arbitrary two-qubit operation, and that exactly half of all controlled-unitary gates have the same uniform upper bound of six applications. This implies that half of the controlled-unitary gates can be used to implement two-qubit operations just as efficiently as the widely used CNOT gate, where efficiency refers to minimizing the uniform upper bound to circuit size. Another important feature of this work is that it suggests a generality beyond the standard model; namely, it offers an efficient *direct* route to simulate any arbitrary two-qubit unitary operation with whatever entangling gates arise naturally in the physical applications.

Preliminary.— We first briefly introduce some basic facts about Cartan decomposition of SU(4) and local equivalence of two-qubit gates. Any two-qubit unitary operation $U \in \mathrm{SU}(4)$ can be decomposed as [8–10]

$$U = k_1 \cdot e^{c_1(i/2)\sigma_x^1\sigma_x^2} \cdot e^{c_2(i/2)\sigma_y^1\sigma_y^2} \cdot e^{c_3(i/2)\sigma_z^1\sigma_z^2} \cdot k_2, \quad (1)$$

where $\sigma_\alpha^1\sigma_\alpha^2 = \sigma_\alpha \otimes \sigma_\alpha$, σ_α are the Pauli matrices, and $k_1, k_2 \in \mathrm{SU}(2) \otimes \mathrm{SU}(2)$ are local gates. The geometric representation of nonlocal gates in [8] defines a set of coefficients c_j satisfying

$$\pi - c_2 \geq c_1 \geq c_2 \geq c_3 \geq 0. \quad (2)$$

Also from [8], we know that local gates $U \in \mathrm{SU}(2) \otimes \mathrm{SU}(2)$ correspond to the case when $c_1 = c_2 = c_3 = 0$, or $c_1 = \pi$, $c_2 = c_3 = 0$; the SWAP gate to $c_1 = c_2 = c_3 = \frac{\pi}{2}$; and the CNOT gate to $c_1 = \frac{\pi}{2}$, $c_2 = c_3 = 0$.

Two unitary transformations $U, U_1 \in \mathrm{SU}(4)$ are called *locally equivalent* if they differ only by local operations: $U = k_1U_1k_2$, where $k_1, k_2 \in \mathrm{SU}(2) \otimes \mathrm{SU}(2)$. It was shown in [8] that any nonlocal two-qubit operation that is not locally equivalent to the SWAP gate is entangling. The SWAP gate and its local equivalence class are thus the only nonlocal two-qubit operations that transform unentangled states to unentangled states, i.e., that do not introduce any entanglement.

Universal quantum circuit.—We now present an analytic way to implement any arbitrary two-qubit gate $U \in \mathrm{SU}(4)$ by constructing a closed form solution for a universal quantum circuit that is composed of a small number of repetitions of a given entangling operation U_g together with local gates. Local gates are assumed to be implementable at ease, as is the case in many of the current proposed physical implementations of quantum computation [2].

An arbitrary two-qubit operation $U \in \mathrm{SU}(4)$ can be written as in Eq. (1). Letting $k_x = e^{(\pi/4)i\sigma_y} \otimes e^{(\pi/4)i\sigma_y}$ and $k_y = e^{(\pi/4)i\sigma_x} \otimes e^{(\pi/4)i\sigma_x}$, we have

$$\sigma_x^1\sigma_x^2 = k_x^\dagger \sigma_z^1\sigma_z^2 k_x, \qquad \sigma_y^1\sigma_y^2 = k_y^\dagger \sigma_z^1\sigma_z^2 k_y. \quad (3)$$

Substituting Eq. (3) into Eq. (1), we find that an arbitrary two-qubit gate $U \in \mathrm{SU}(4)$ can be written as

$$U = (k_1k_x^\dagger)e^{c_1(i/2)\sigma_z^1\sigma_z^2}(k_xk_y^\dagger)e^{c_2(i/2)\sigma_z^1\sigma_z^2}(k_y)e^{c_3(i/2)\sigma_z^1\sigma_z^2}(k_2), \quad (4)$$

where k_1, k_2, k_x, and k_y are all local gates. Since we have all the local gates at our full disposal, it is evident that we need only to implement the nonlocal block $e^{c_j(i/2)\sigma_z^1\sigma_z^2}$ from the given entangling gate U_g together with local gates, for general values of c_j between 0 and $\pi/2$. We have found the following analytic construction of this general block.

Step 1. Apply U_g at most twice to build a gate $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$ with $\gamma \in (0, \frac{\pi}{2}]$ (Proposition 1). The value of γ obtained depends on the starting U_g.

Step 2. Apply $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$ n times, until $n\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$.

Step 3. Apply $e^{n\gamma(i/2)\sigma_z^1\sigma_z^2}$ with $n\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$ twice, to simulate the nonlocal block $e^{c_j(i/2)\sigma_z^1\sigma_z^2}$ (Proposition 2).

Step 4. Build the quantum circuit according to Eq. (4).

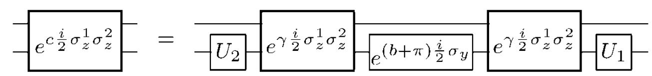
We now describe this construction in more detail.

Proposition 1.—Any arbitrary given entangling gate U_g can simulate a gate $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$, where $\gamma \in (0, \frac{\pi}{2}]$, by a quantum circuit that applies U_g at most twice.

The proof is provided in [11].

Now it is evident that if the constructed gate $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$ has $\gamma \in (0, \frac{\pi}{4}]$, then it can be applied for n times until $n\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$ (Step 2). In the next Proposition, we will use the resulting gate $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$ with $\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$, as a basic building block to simulate any generic nonlocal block $e^{c(i/2)\sigma_z^1\sigma_z^2}$ (Step 3). Without loss of generality, we need only to consider the case when $c \in (0, \frac{\pi}{2}]$.

Proposition 2.—Given a gate $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$, where $\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$, together with local gates, the following quantum circuit can simulate the gate $e^{c(i/2)\sigma_z^1\sigma_z^2}$ for any $c \in (0, \frac{\pi}{2}]$:



In the above quantum circuit, we have

$$U_1 = \begin{pmatrix} ip & iq \\ -q & p \end{pmatrix}, \qquad U_2 = \begin{pmatrix} ip & -q \\ -iq & -p \end{pmatrix}, \quad (5)$$

$$b = \cos^{-1}[(\cos c - \cos^2\gamma)/\sin^2\gamma], \quad (6)$$

where

$$p = \sqrt{\frac{1}{2}\left(1 + \frac{\tan\frac{c}{2}}{\tan\gamma}\right)}, \qquad q = \sqrt{\frac{1}{2}\left(1 - \frac{\tan\frac{c}{2}}{\tan\gamma}\right)}. \quad (7)$$

Proof.—We first justify the condition $\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$. From Eq. (6), we have $\cos c = \sin^2\gamma\cos b + \cos^2\gamma$. Therefore, $\cos 2\gamma \leq \cos c \leq 1$, which yields $0 \leq c \leq 2\gamma$. To cover the full range $(0, \frac{\pi}{2}]$ of c, we therefore require that $\gamma \geq \frac{\pi}{4}$.

We now derive a few formulas required for the proof below. It is straightforward to show that $p^2 + q^2 = 1$. The identity $\sin\frac{c}{2} = \sin\gamma\sin\frac{b}{2}$ follows from Eq. (6) by direct derivations. This yields

$$\tan^2\gamma = \frac{\sin^2\frac{c}{2}}{\sin^2\frac{b}{2} - \sin^2\frac{c}{2}},$$

whence

$$pq = \frac{1}{2}\sqrt{1 - \frac{\tan^2\frac{c}{2}}{\tan^2\gamma}} = \frac{\cos\frac{b}{2}}{2\cos\frac{c}{2}}. \quad (8)$$

The Proposition can now be proved. Since $p^2 + q^2 = 1$, it is easy to see that $U_1U_1^\dagger = U_2U_2^\dagger = I$. Hence, U_1 and U_2 are indeed single-qubit gates. The quantum circuit can be rewritten as

$$(I \otimes U_1)e^{\gamma(i/2)\sigma_z^1\sigma_z^2}(I \otimes e^{(b+\pi)(i/2)\sigma_y})e^{\gamma(i/2)\sigma_z^1\sigma_z^2}(I \otimes U_2) = \begin{pmatrix} W & \\ & V \end{pmatrix}, \tag{9}$$

where

$$W = U_1 \cdot e^{i(\gamma/2)\sigma_z} \cdot e^{(b+\pi)(i/2)\sigma_y} \cdot e^{i(\gamma/2)\sigma_z} \cdot U_2, \tag{10}$$

$$V = U_1 \cdot e^{-i(\gamma/2)\sigma_z} \cdot e^{(b+\pi)(i/2)\sigma_y} \cdot e^{-i(\gamma/2)\sigma_z} \cdot U_2. \tag{11}$$

After substituting Eq. (5) into Eq. (10) and applying the identities $\sin\frac{c}{2} = \sin\gamma \sin\frac{b}{2}$ and Eq. (8), we obtain

$$W_{11} = p^2 \sin\frac{b}{2}e^{i\gamma} + 2pq\cos\frac{b}{2} - q^2\sin\frac{b}{2}e^{-i\gamma} = e^{c(i/2)},$$
$$W_{22} = p^2 \sin\frac{b}{2}e^{-i\gamma} + 2pq\cos\frac{b}{2} - q^2\sin\frac{b}{2}e^{i\gamma} = e^{-c(i/2)},$$
$$W_{12} = W_{21} = 2ipq\sin\frac{b}{2}\cos\gamma - i(p^2 - q^2)\cos\frac{b}{2} = 0.$$

Hence, $W = e^{c(i/2)\sigma_z}$. Similarly, we find $V = e^{-c(i/2)\sigma_z}$. Equation (9) now becomes

$$(I \otimes U_1)e^{\gamma(i/2)\sigma_z^1\sigma_z^2}(I \otimes e^{(b+\pi)(i/2)\sigma_y})e^{\gamma(i/2)\sigma_z^1\sigma_z^2}(I \otimes U_2) = \begin{pmatrix} e^{c(i/2)\sigma_z} & \\ & e^{-c(i/2)\sigma_z} \end{pmatrix} = e^{c(i/2)\sigma_z^1\sigma_z^2},$$

which completes the proof. ■

Note that in the above Proposition, for the extreme case when $\gamma = \frac{\pi}{2}$, corresponding to starting from a CNOT gate, we have $b = c$, and

$$U_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} i & i \\ -1 & 1 \end{pmatrix}, \qquad U_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} i & -1 \\ -i & -1 \end{pmatrix}.$$

As a physical example, let us consider neutral atoms in an optical lattice as a simulator for a solid state many-body spin system. The simulation objective may, for instance, be implementation of $\sqrt{\mathrm{SWAP}}$. While this is readily generated in spin systems, from the isotropic exchange Hamiltonian [12], it is not directly accessible for neutral atoms in optical lattices. A convenient experimentally accessible nonlocal transformation in this setting is the controlled-PHASE gate C_ϕ, where the PHASE gate is $\begin{pmatrix} 1 & \\ & e^{i\phi} \end{pmatrix}$. From the Cartan decomposition, we have

$$C_\phi = e^{i(\phi/4)} \cdot e^{-i(\phi/4)\sigma_z} \otimes e^{-i(\phi/4)\sigma_z} \cdot e^{(\phi/2)(i/2)\sigma_z^1\sigma_z^2}. \tag{12}$$

On the other hand, the $\sqrt{\mathrm{SWAP}}$ gate can be written as

$$\sqrt{\mathrm{SWAP}} = e^{-i(\pi/8)} \cdot e^{(\pi/4)(i/2)\sigma_x^1\sigma_x^2} \cdot e^{(\pi/4)(i/2)\sigma_y^1\sigma_y^2} \cdot e^{(\pi/4)(i/2)\sigma_z^1\sigma_z^2}.$$

From the quantum circuit in Eq. (4), since $c_1 = c_2 = c_3 = \frac{\pi}{4}$, we need only to implement the nonlocal gate $e^{(\pi/4)(i/2)\sigma_z^1\sigma_z^2}$. For $\phi \in [\frac{\pi}{2}, \pi]$, from Proposition 2 and Eq. (12), we get

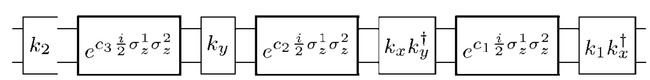
$$e^{(\pi/4)(i/2)\sigma_z^1\sigma_z^2} = e^{-i(\phi/2)} \cdot (e^{i(\phi/4)\sigma_z} \otimes U_1 e^{i(\phi/4)\sigma_z}) \cdot C_\phi \cdot (e^{i(\phi/4)\sigma_z} \otimes e^{(i/2)(b+\pi)\sigma_y}e^{i(\phi/4)\sigma_z}) \cdot C_\phi \cdot (I \otimes U_2),$$

where $b = \cos^{-1}[(\frac{1}{\sqrt{2}} - \cos^2\frac{\phi}{2})/\sin^2\frac{\phi}{2}]$, U_1 and U_2 are given as in Eq. (5), and

$$p = \sqrt{\frac{1}{2}\left(1 + \frac{\sqrt{2}-1}{\tan\frac{\phi}{2}}\right)}, \qquad q = \sqrt{\frac{1}{2}\left(1 - \frac{\sqrt{2}-1}{\tan\frac{\phi}{2}}\right)}.$$

Thus, a spin-spin interaction can be simulated in an optical lattice with only two repetitions of a controlled-PHASE gate C_ϕ having $\phi \in [\frac{\pi}{2}, \pi]$.

Uniform upper bound.—One often desires to simulate an arbitrary two-qubit operation by applying the given entangling two-qubit operation as infrequently as possible. From the construction procedure described above, we first use the given entangling gate U_g to implement a gate $U_f = e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$ with $\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$ (Proposition 1), and then apply U_f twice, to implement a generic nonlocal gate $e^{c(i/2)\sigma_z^1\sigma_z^2}$ (Proposition 2). From the decomposition of SU(4) in Eq. (4), any arbitrary two-qubit unitary operation contains at most three such nonlocal blocks, resulting in the quantum circuit

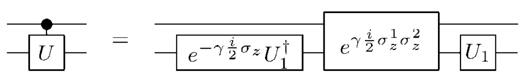


where each nonlocal block $e^{c_j(i/2)\sigma_z^1\sigma_z^2}$ is simulated as shown in the circuit of Proposition 2. It is clear that overall we only need to apply the gate U_f at most six times, in order to simulate an arbitrary two-qubit operation. We thereby obtain an *upper bound* for the applications of the given entangling gate U_g to construct an exact universal quantum circuit. The value of this upper bound depends only on the nonlocal part of the given gate. For example, for a controlled-PHASE gate C_ϕ with parameter $\phi \in [\frac{\pi}{2}, \pi]$, it takes six applications of C_ϕ and seven local gates to simulate any arbitrary two-qubit operation. However, when $\phi \in (0, \frac{\pi}{2})$, we first need to apply C_ϕ n times until $n\phi \geq \frac{\pi}{2}$. Consequently, in this case it takes $6n$ applications of C_ϕ and $6n + 1$ local gates to implement any arbitrary two-qubit operation. Furthermore, this upper bound is uniform in the sense that no matter which two-qubit unitary operation is to be implemented, we can always construct a quantum circuit to simulate this operation with applications of the given entangling gate U_g not exceeding the upper bound.

It is instructive to compare these results with the numerical solution for construction of CNOT obtained in [7]. For the gate $U_g = e^{(\pi/3)(i/2)\sigma_z^1\sigma_z^2}$, both procedures need only two applications to obtain the CNOT gate. When $U_g = e^{(\pi/5)(i/2)\sigma_z^1\sigma_z^2}$, our uniform construction requires four applications, whereas the procedure of [7] needs only three applications to get CNOT. This difference derives from the fact that our procedure provides a uniform solution and is not optimized for any specific gate, whereas the procedure of [7] is near optimal for CNOT. This comparison reveals that the uniform property and optimality cannot necessarily be satisfied simultaneously.

Our final analysis concerns the efficiency of these analytic circuits. We first show that our basic building blocks of the quantum circuit, namely, the gates $e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$, are locally equivalent to the controlled-unitary (controlled-U) gates.

Proposition 3.—Consider an arbitrary single-qubit gate $U = \exp\{i\gamma\hat{n}\cdot\vec{\sigma}\}$, *where* $\gamma \in \mathbb{R}^+$, $\hat{n} = (n_x, n_y, n_z)$ *is a unit vector in* $\mathbb{R}^3$, *and* $\vec{\sigma}$ *denotes the vector* $(\sigma_x, \sigma_y, \sigma_z)$ *of Pauli matrices. The corresponding controlled-U gate can be simulated by the following quantum circuit:*



where

$$U_1 = \begin{cases} \begin{pmatrix} i\sqrt{\frac{1-n_z}{2}} & \sqrt{\frac{1+n_z}{2}} \\ \frac{n_y - n_x i}{\sqrt{2(1-n_z)}} & \frac{n_x + n_y i}{\sqrt{2(1+n_z)}} \end{pmatrix}, & \text{for } n_z \neq \pm 1; \\ \sigma_x, & \text{for } n_z = 1; \\ I, & \text{for } n_z = -1. \end{cases}$$

This proposition can be proved by substitution of U_1, followed by direct algebraic computation [11].

We saw above that all the gates $U_f = e^{\gamma(i/2)\sigma_z^1\sigma_z^2}$ with $\gamma \in [\frac{\pi}{4}, \frac{\pi}{2}]$ have the same upper bounds. When $\gamma = \frac{\pi}{2}$, U_f is locally equivalent to the CNOT gate. From [8], there exists a one-to-one map from the local equivalence classes of controlled-U gates to the points in the interval $[0, \frac{\pi}{2}]$. Furthermore, those gates having the same upper bounds as the CNOT gate constitute half of this interval, namely, $[\frac{\pi}{4}, \frac{\pi}{2}]$. Therefore, using the length of the interval as a measure, we conclude that *exactly half* of the controlled-U gates can be used to construct universal quantum circuits that satisfy the same upper bound, i.e., they can be used just as efficiently as the CNOT gate. (Note that this is true despite the fact that CNOT is the only controlled-U gate providing perfect entanglement [8].) Consequently, there is no need to restrict practical studies of physical implementation of quantum circuits for universal computation or for quantum simulations to the standard model of CNOT with local gates.

In summary, we have provided an analytic approach to construct a universal quantum circuit that can simulate any arbitrary two-qubit operation given any entangling gate U_g supplemented with local gates. Closed form solutions have been derived for each step in this explicit construction procedure. The procedure was illustrated on a physical example of simulation of a solid state spin system with neutral atoms in an optical lattice. Our approach provides a uniform upper bound for the applications of the given entangling gate U_g. It was found that precisely half of all the controlled-U gates have the same uniform upper bounds as the CNOT gate. This offers new options for realization of interactions in simulation of one quantum many-body system by another, as well as for efficient implementation of quantum computation.

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