Optimal Quantum Circuits for General Two-Qubit Gates

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In order to demonstrate non-trivial quantum computations experimentally, such as the synthesis of arbitrary entangled states, it will be useful to understand how to decompose a desired quantum computation into the shortest possible sequence of one-qubit and two-qubit gates. We contribute to this effort by providing a method to construct an optimal quantum circuit for a general two-qubit gate that requires at most 3 CNOT gates and 15 elementary one-qubit gates. Moreover, if the desired two-qubit gate corresponds to a purely real unitary transformation, we provide a construction that requires at most 2 CNOTs and 12 one-qubit gates. We then prove that these constructions are optimal with respect to the family of CNOT, y-rotation, z-rotation, and phase gates.

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I. INTRODUCTION

It is known that any n-qubit quantum computation can be achieved using a sequence of one-qubit and two-qubit quantum logic gates [1, 2]. However, even for two-qubit gates, finding the optimal circuit with respect to a particular family of gates is not easy [3]. This is unfortunate because, at the current time, quantum computer experimentalists can only achieve a handful of gate operations within the coherence time of their physical systems [4]. Without a procedure for optimal quantum circuit design, experimentalists might be unable to demonstrate certain quantum computational milestones even though they ought to be within reach. For example, a current experimental goal is the synthesis of any two-qubit entangled state [5]. Although it is known, in principle, how to synthesize any such state [6], the resulting quantum circuits can be suboptimal, requiring excessive numbers of CNOT gates, if done judiciously [7]. The current solution to this problem uses rewrite rules to recognize and eliminate redundant gates. However, a better solution would be to perform optimal design from the outset.

In this paper we give a procedure for constructing an optimal quantum circuit for achieving a general two-qubit quantum computation, up to a global phase, which requires at most 3 CNOT gates and 15 elementary one-qubit gates from the family $fR_y, fR_z g$. We prove that this construction is optimal, in the sense that there is no smaller circuit, using the same family of gates, that achieves this operation. In addition, we show that if the unitary matrix corresponding to our desired gate is purely real, it can be achieved using at most 2 CNOT gates and 12 one-qubit gates.

A flurry of recent results on gate-count minimization for general two-qubit gates, report similar findings to us. Vidal and Dawson proved that 3 CNOTs are sufficient to implement a general $U \in SU(4)$ and that two-qubit controlled-V operations require at most 2 CNOTs [8]. Vatan and Williams proved that any $U \in SU(4)$ requires at most 3 CNOTs, and 16 elementary one-qubit $fR_y, fR_z g$ gates, that any $U \in SO(4)$ (i.e., real gate) requires at most 2 CNOTs and 12 one-qubit $fR_y, fR_z g$ gates, and that these constructions are optimal [9]. Later, Shende, Markov, and Bullock reported similar results on circuit complexity for $U \in SU(4)$, and specialized the complexity bounds depending on which families of one-qubit gates were being used [10]. Fundamentally, all these results rest upon the decompositions of a general $U \in SU(4)$ given in [11, 12] and used in the GQC quantum circuit compiler [13].

The remainder of the paper is organized as follows. After introducing some notation in Section II, we discuss the magic basis [11] in Section III and prove (in Theorems 1 and 2) its most important property, namely, that real entangling two-qubit operations become non-entangling in the magic basis. We also prove (via the circuit shown in Fig. I) that the magic basis transformations require at most one CNOT to implement them explicitly. This is in contrast to Fig. 3 in [15], which required three CNOTs. It turns out that this compact quantum circuit for the magic basis transformation is the cornerstone of our subsequent constructions for generic two-qubit gates, and our proofs of their optimality. In Section IV we present the first such construction, which proves that any two-qubit gate in $SO(4)$ can be implemented in 12 elementary (i.e., $R_y, R_z$) gates and 2 CNOTs. Theorem IV extends this results to any two-qubit gate in $O(4)$ with determinant equal to 1, and proves that any such gate requires 12 elementary gates and 3 CNOTs. In Section V these results are generalized to the generic two-qubit gates in $U(4)$, and we provide an explicit construction that requires 15 elementary gates and 3 CNOTs. Finally, in Section VI we prove that our construction for generic two-qubit gates is optimal by showing that there is at least one gate in $U(4)$, namely the two-qubit SWAP gate, which cannot be implemented in fewer than 3 CNOTs.

II. NOTATION

Throughout this paper we identify a quantum gate with the unitary matrix that defines its operation. We take rotations about the y and z-axes, respectively $R_y(\cdot)$ and $R_z(\cdot)$, as our
elementary one-qubit gates; i.e.,

\[ R_y(\theta) = \begin{bmatrix} \cos \frac{\theta}{2} & i \sin \frac{\theta}{2} \\ \sin \frac{\theta}{2} & \cos \frac{\theta}{2} \end{bmatrix} ; \quad R_z(\theta) = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix} \]

However, we also have three special one-qubit gates: the one-qubit identity matrix \( \mathbb{1}_k \), and the Hadamard gate \( H \) and the phase gate \( S \) defined as

\[ H = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} ; \quad S = \begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix} \]

We define two CNOT gates, CNOT1 a standard CNOT gate with the control on the top qubit and the target on the bottom qubit, and CNOT2 with the control and target qubits flipped. Thus

\[ \text{CNOT1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} ; \quad \text{CNOT2} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \]

We also use the two-qubit gate SWAP gate, which is defined as

\[ \text{SWAP} = \text{CNOT1} \quad \text{CNOT2} \quad \text{CNOT1} \]

We use the notation the ^\_\_1(\upsilon) for the controlled-V gate, where \( \upsilon \in U(2) \). Throughout this paper we assume that for the ^\_\_1(\upsilon) gate the control qubit is the first (top) qubit. Therefore,

\[ ^\_\_1(\upsilon) = \mathbb{1}_k \quad \upsilon \]

In the special case of the ^\_\_1(\upsilon) gate, we use the notation CZ. For any unitary matrix \( U \), we denote its inverse, i.e., the conjugate-transpose of \( U \), by \( U^\dagger \).

III. MAGIC BASIS

There are different ways to define the magic basis \[ \mathbb{1}_2 \[ \mathbb{1}_2 \[ \mathbb{1}_2 \]. Here we use the definition used in \[ \mathbb{1}_2 \[ \mathbb{1}_2 \[ \mathbb{1}_2 \].

\[ M = \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & i \\ 1 & i & 0 \end{bmatrix} \]

The circuit of FIG.\[ \text{II} \]implementes this transformation.

The following theorem presents the basic property of the magic basis. This result is already known (see, e.g., \[ \mathbb{1}_2 \[ \mathbb{1}_2 \[ \mathbb{1}_2 \]), and we provide a proof for the sake of completeness.

**Theorem 1.** For every real orthogonal matrix \( U \in SO(4) \), the matrix of \( U \) in the magic basis, i.e., \( M = U \cdot M \) is tensor product of two 2-dimensional special unitary matrices. In other words: \( M = U \cdot M \in SU(2) \cdot SU(2) \).

**Proof.** Proof. We prove the theorem by showing that for every \( A \cdot B \in SU(2) \cdot SU(2) \), we have \( M = A \cdot B \cdot M \in SO(4) \).

It is well-known that every matrix \( A \in SU(2) \) can be written as the product \( R_x(\theta) \cdot R_y(\phi) \cdot R_z(\gamma) \), for some \( \theta, \phi, \gamma \). Therefore any matrix \( A \cdot B \in SU(2) \cdot SU(2) \) can be written as a product of the matrices of the form \( V \cdot \mathbb{1}_k \cdot V \), where \( V \) is either \( R_y(\phi) \) or \( R_z(\gamma) \). Thus the product is complete if \( V \cdot \mathbb{1}_k \cdot V \cdot M \), and \( M \cdot \mathbb{1}_k \cdot V \cdot M \), are in \( SO(4) \). Elementary algebra shows that this the case.

Since the mapping \( A \cdot B \in SU(2) \cdot SU(2) \) is one-to-one and the spaces \( SU(2) \cdot SU(2) \) and \( SO(4) \) have the same topological dimension, we conclude that this mapping is an isomorphism between these two spaces.

Note that the above theorem is not true for all orthogonal matrices in \( O(4) \). In fact, for every matrix \( U \in O(4) \), either \( \det(U) = 1 \) or \( \det(U) = -1 \) for which the above theorem holds, or \( \det(U) = 1 \) for which we have the following theorem.

**Theorem 2.** For every \( U \in O(4) \) with \( \det(U) = 1 \), the matrix \( M = U \cdot M \) is a tensor product of 2-dimensional unitary matrices and one SWAP gate in the form of the following decomposition: \( M = U \cdot M = A \cdot B \cdot \text{SWAP} \cdot \mathbb{1}_k \cdot z \); where \( A \cdot B \in U(2) \).

**Proof.** First note that \( \det(CNOT1) = 1 \) and \( \det(U \cdot CNOT1) = 1 \). Then \( M \cdot CNOT1 \cdot M = S \cdot S \cdot \text{SWAP} \cdot \mathbb{1}_k \cdot z \). Since \( M \cdot U \cdot M = M \cdot U \cdot CNOT1 \cdot M = CNOT1 \cdot M \cdot CNOT1 \cdot M \), the theorem follows from Theorem \[ \text{II} \]

IV. REALIZING TWO-QUBIT GATES FROM O(4)

Let \( U \in SO(4) \). Then Theorem \[ \text{II} \] shows that \( M = A \cdot B \), where \( A \cdot B \in SU(2) \). Therefore, \( U = M \cdot A \cdot B \cdot M \). We use the circuit of Fig.\[ \text{II} \] for computing the magic basis transform \( M \) to obtain a circuit for computing the unitary operation \( U \). This circuit can be simplified by using the decompositions \( S = e^{i\frac{\pi}{4}} R_x(\frac{\pi}{2}) \) and \( H = R_y(\frac{\pi}{2}) \). Note that \( \mathbb{1}_k \cdot z \) and the CNOT2 gates commute, and the overall phases \( e^{i\frac{\pi}{4}} \) and \( e^{i\frac{\pi}{4}} \) from \( S \) and \( H \) cancel out. Hence we obtain the circuit of Fig.\[ \text{II} \] for computing a general two-qubit gate from \( SO(4) \). Thus we have proved the following theorem.

**Theorem 3.** Every two-qubit quantum gate in \( SO(4) \) can be realized by a circuit consisting of 12 elementary one-qubit gates and 2 CNOT gates.
Next, we generalize these results to construct circuits for gates from $O(4)$ with determinant equal to 1.

**Theorem 4.** Every two-qubit quantum gate in $O(4)$ determinant equal to 1 can be realized by a circuit consisting of 12 elementary gates and 2 CNOT gates and one SWAP gate (see FIG. 3).

Next, we generalize these results to construct circuits for gates in $U(4)$.

**V. REALIZING TWO-QUBIT GATES FROM $U(4)$**

In is known that every $U \in U(4)$ can be written as

$$U = A_1 \; A_2 \; N \; A_3 \; A_4$$

where $A_j \in U(2)$ and

$$N \; \{ \; i,j \; \} = \exp \{ \pi \; \langle x \; x + y \; y + z \; z \rangle \}$$

for $i,j \in \mathbb{R}$ (see, e.g., $[11, 12, 13]$). Note that if $U \in SU(4)$, then we can choose all operations $A_j$ in $SU(2)$. Our construction is based on constructing an optimal circuit for computing $N \; \{ \; i,j \; \}$. To this end, we first note that $D = M \; N \; M$ is a diagonal matrix of the form

$$\text{diag} \; e^{i (x + y + z)}; e^{i (x + y + z)}; e^{i (x + y + z)}.$$ Therefore, $N \; \{ \; i,j \; \} = \frac{1}{2} \; M \; D \; M$. Utilizing the circuit of FIG. 11 for $M$, we get the circuit of FIG. 12 for computing $N \; \{ \; i,j \; \}$. Note that $S \; S \; D \; S \; S = D$. Then we substitute the right-hand side Hadamard gate of FIG. 4 by 3 gates, using the following identity: $1 \text{H} = CNOT1 \; \text{H} = \text{CZ}$. Now, the matrix $D = \text{CZ} \; D$ is a diagonal matrix, and

$$\text{(1)} \; \text{H} = \text{CNOT1} \; \text{H} = \text{CZ}.$$  

where

$$V_1 = e^{i \; \cos(\tau)} \; e^{i \; \sin(\tau)} ; \quad e^{i \; \cos(\tau)} ; \quad e^{i \; \sin(\tau)} ;$$

$$V_2 = e^{i \; \cos2(\tau)} \; e^{i \; \sin2(\tau)} ; \quad e^{i \; \cos2(\tau)} ; \quad e^{i \; \sin2(\tau)} ;$$

We have the following decompositions for $V_1$ and $V_2$ (see also $[7]$):

$$V_1 = e^{i \; \cos(\tau)} \; G \; e^{i \; \sin(\tau)} ; \quad \text{R}_x (\tau) ;$$

and

$$V_2 = e^{i \; \cos2(\tau)} \; G \; e^{i \; \sin2(\tau)} ; \quad \text{R}_x (\tau) ; \quad \text{R}_y (\tau) ;$$

By utilizing the equations (2)–(4), we can convert the circuit of FIG. 4 to the circuit of FIG. 5.

![FIG. 5: A circuit for implementing $N \; \{ \; i,j \; \}$; second version. Here $S_1 = R_z (\tau)$, $S_2 = R_x (\tau)$, $T_1 = R_y (\tau \; 2 \; \tau)$, and $T_2 = R_y (\tau \; 2 \; \tau)$.

Now we focus on the sequence $\text{CNOT1} \; \text{CNOT1}$ of operations. We have the following identity

$$\text{CNOT1} \; \text{CNOT1} = \text{CNOT2} \; \text{R}_z (\tau) \; \text{CNOT1}.$$ 

After applying this rule, the two consecutive CNOT2 gates on the right-hand side of the circuit reduce to the identity. Also note that, on the left-hand side of the circuit, we can apply the rule

$$\text{CNOT1} \; \text{R}_z (\tau) \; \text{CNOT1} = \text{CNOT1} \; \text{CNOT1} \; \text{R}_z (\tau) ;$$

Thus the circuit of FIG. 5 can be converted to the circuit of FIG. 7. Note that the operation defined by this circuit has determinant equal to 1, thus we need to add a global $e^{i \; \pi}$ phase to get the special unitary operation $N \; \{ \; i,j \; \}$ exactly. Now utilizing the circuit of FIG. 7 and the canonical decomposition of $D$, we could get a circuit to realize the operation $U \in U(4)$.

Note that in this process, the left and right-hand side operations $R_z (\tau)$ and $R_z (\tau)$ of FIG. 5 will be “absorbed” by adjacent $A_j$. The final result is the circuit of FIG. 5 and we have proved the following theorem.
Theorem 5. Every two-qubit quantum gate in $U(4)$ can be realized, up to a global phase, by a circuit consisting of 15 elementary one-qubit gates and 3 CNOT gates.

VI. THREE CNOT GATES ARE NEEDED

To show that the construction of Theorem 5 is optimal, we prove that there is at least one gate in $U(4)$, namely the two-qubit SWAP gate, a real unitary matrix having a determinant of 1, which requires no less than 3 CNOT gates.

In the proof of the following theorem we utilize the notion of entangling power introduced in [17]. For a unitary operation $U \in U(4)$, the entangling power of $U$ is defined as

$$\text{EP}(U) = \text{average } E_{j_1 i_1 j_2 i_2}$$

where average is over all product states $j_1 i_1 j_2 i_2$ and $C^2$ distributed according to the uniform distribution (in general, we can define EP with regards to any distribution, but here we only consider the uniform distribution). In the above formula $E$ is the linear entropy entanglement measure defined for $j_1 i_2 C^4$ as follows:

$$E_{j_1 i_2} = \text{tr}_{i_2}^2;$$

where $\text{tr}_{i_2}$ is the result of tracing out the $i_2$th qubit. Note that $E_{j_1 i_2} = \frac{1}{2}$, and the lower or upper bound is obtained if $j_1 i_2$ is a product state or a maximally entangled state, respectively. In [17] the following simple formula for calculating EP is presented:

$$\text{EP}(U) = \frac{3}{2} \frac{1}{3^6} U^2 T_{113} U^2 T_{113} + (\text{SWAP } U^2 T_{113} \text{SWAP } U^2 T_{113};$$

where the Hilbert-Schmidt scalar product $hA;B$ is defined as $hA;B = \text{tr}(A^T B)$ and the permutation $T_{113}$ on $C^2 \otimes C^2$ is the transposition $T_{113} b_1b_2c_1c_2d_1 = b_2b_1c_1c_2d_1$ on the system of 4 qubits.

We will utilize the following basic properties of the function EP.

For every $U \in U(4)$ we have $0 \leq \text{EP}(U) \leq \frac{5}{2}$.

For every $A ; B \in U(2)$ we have $\text{EP}(A ; B) = 0$.

For every $U \in U(4)$ and $A ; B \in U(2)$ we have $\text{EP}(A ; B) U = \text{EP}(U) \cdot (A ; B)$.

$\text{EP}(U) = \text{EP}(U^0)$.

$\text{EP}(\text{SWAP}) = \frac{4}{2}$ and $\text{EP}(\text{SWAP}) = 0$.

We will also use the simple fact that $\text{SWAP}$ cannot be written as $\text{SWAP} = A ; B$, where $A ; B \in U(2)$.

Theorem 6. To compute the SWAP at least 3 CNOT gates are needed.

Proof. We construct a proof by contradiction. Suppose that there is a circuit computing SWAP and consists of less than three CNOT gates. We consider two possible cases.

Case 1. Suppose that SWAP is computed by a circuit consisting of two CNOT gates. We substitute each CNOT gate by a small subcircuit in terms of CZ (controlled-$\pi$) gate; i.e.,

$$\text{CNOT} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \text{H} \text{CZ} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \text{H}.$$ 

Then by utilizing the following commutation rules

$$\text{CZ} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{R}_Z(t) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{R}_Z(t) \text{CZ};$$

$$\text{CZ} \text{R}_Z(t) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = \text{R}_Z(t) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \text{CZ};$$

we obtain the simplified circuit of FIG. 3 for computing the SWAP gate. Note that in this figure we choose the top (first) qubit as the control qubit for the CZ gates, but we could choose the other qubit as the control qubit as well, since the action of the CZ gate is not change by switching the control and target qubits. Now, let

$$U = \text{CZ} \text{R}_Y(a) \text{R}_Y(b) \text{CZ};$$
Then
\[ \text{EP}(U) = \text{EP}(\text{SWAP}) = \frac{1}{2}(3 \cos(2a) \cos(2b) \cos(2a) \cos(2b)) = 0: \]

Therefore, \( a \neq b \neq \frac{\pi}{2} \neq \theta \). Thus we have the following four possible cases for the unitary operation \( U \):

- If \( a = b = 0 \), then \( U = \text{I} \);
- If \( a = 0, b = \theta \), then \( U = \text{R}_y(\theta) \);
- If \( a = \theta, b = 0 \), then \( U = \text{R}_y(\theta) \);
- If \( a = b = \theta \), then \( U = \text{R}_x \).

In each case, we conclude that \( \text{SWAP} = V_1 V_2 \), for some \( V_1, V_2 \in U(2) \), which is a contradiction.

**Case 2.** Suppose that \( \text{SWAP} \) is computed by a circuit consisting of only one CNOT gate; for example

\[ \text{SWAP} = A_1 A_2 \text{ CNOT} A_3 A_4; \]

where \( A_j \in U(2) \). Then \( \text{EP}(\text{SWAP}) = \text{EP}(\text{CNOT}) \), which again is a contradiction.

**VII. CONCLUSION**

In this paper we prove tight bounds on the numbers of one-qubit gates and CNOT gates needed to implement generic two-qubit quantum computations. In addition, we give a constructive procedure for finding such decompositions, which uses the Kraus-Cirac decomposition to find the core entangling operation underlying the two-qubit gate, i.e., \( N(\; ; \;) \), and then substitutes the discovered parameter values into an equivalent circuit template for \( N(\; ; \;) \) as shown in Fig. 8. The net result is an explicit circuit for any desired two-qubit unitary operation that uses at most three CNOTs and 15 elementary \( y \)- or \( z \)-single qubit rotations.

We point out that it is possible to decompose a desired unitary operation into many different families of quantum gates. For example, the basis of all one-qubit gates augmented with CNOT was first studied in [2], and was shown to be capable of implementing any \( n \)-qubit unitary operation exactly. This scheme has the advantage that only a single, fixed, type of two-qubit gate need be built. Similar schemes are known that use different fixed entangling operations such as \( \text{SWAP} \) gates (in superconducting quantum computing) and \( \text{CZ} \) gates (in spintronic quantum computing). In addition, other decompositions are possible that use parameterized two-qubit gates. These may lead to more efficient factorizations in special cases, but also make for a more complicated quantum computer architecture.

The motivation for our work comes from the fact that it is still very difficult, experimentally, to implement multiple quantum gates. Thus, in order to attain near term experimental milestones, it will be important to minimize the number of gates they require. Although our scheme yields minimal circuits for generic two qubit operations, further reductions are still possible in certain special cases. We therefore augment our procedure with rewrite rules, to find even simpler circuits if they exist. Hence, our new construction brings certain state synthesis tasks within the grasp of experimentalists.

In addition, as quantum circuits for (arbitrary) \( n \)-qubit operations are always expressed in terms of a sequence of one-qubit and two-qubit gates, by designing component two-qubit operations minimally, we can sometimes improve the efficiency of implementing \( n \)-qubit computations.

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