How many CNOT gates does it take to generate a three-qubit state?

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The number of two-qubit gates required to transform deterministically a three-qubit pure quantum state into another is discussed. We show that any state can be prepared from a product state using at most three CNOT gates, and that, starting from the GHZ state, only two suffice. As a consequence, any three-qubit state can be transformed into any other using at most four CNOT gates. Generalizations to other two-qubit gates are also discussed.

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Quantum information and computation (see e.g. [1]) is usually described using qubits as elementary units of information which are manipulated through quantum operators. In most practical implementations, such operators have to be realized as sequences of local transformations acting on a few qubits at a time. Whereas one-qubit gates alone cannot create entanglement, it has been shown that together with two-qubit gates they can form universal sets, from which the set of all unitary transformations of any number of qubits can be generated [2]. The complexity of a quantum algorithm is usually measured by assessing the number of elementary gates needed to perform the computation. The Controlled-Not (CNOT) gate, a two-qubit gate whose action can be written \(|00\rangle \rightarrow |00\rangle, |01\rangle \rightarrow |01\rangle, |10\rangle \rightarrow |11\rangle, |11\rangle \rightarrow |10\rangle\), is one of the most widely used both for theory and implementations. It can be shown that the CNOT gate together with one-qubit gates is a universal set [2]. Experimental implementations of a CNOT gate (or the equivalent controlled phase-flip) have been recently reported using e.g. atom-photon interaction in cavities [3], linear optics [4], superconducting qubits [5, 6] or ion traps [7, 8]. While large size quantum computers are still far away, small platforms of a few qubits exist or can be envisioned in the framework of these existing experimental techniques. In most such implementations, two-qubit gates such as the CNOT are much more demanding that one-qubit gates. Theoretical quantum computation has been usually focused on assessing the number of elementary gates to build a given unitary operator performing a given computation. Some works have tried to focus on two-qubit gates and to minimize their number in order to build a given unitary transformation for several qubits [9, 10]. Still, unitary transformations in many applications are a tool to transform an initial state to a given state. It seems therefore natural to try and assess how costly this process is in itself. In this paper, we thus study the minimal number of two-qubit gates needed to change a given quantum state to obtain another one. Of course, this number is necessarily upper bounded by the number required for a general unitary transformation. We focus on the case of two and three qubits. For two qubits, we generalize the result of [11] and show that one CNOT is enough to go from any given pure state to any other one. For three qubits, we show that three CNOTs are enough to go from \(|000\rangle\) to any other pure state, and that two CNOTs suffice if one starts from the GHZ state \(((000) + |111\rangle)/\sqrt{2}\). A corollary of the latter is thus that four CNOTs are enough to go from any pure state to any other pure state. The number of CNOT gates required to go from a state to another defines a discrete distance on the Hilbert space. Given any fixed state \(|\psi\rangle\), the Hilbert space can be partitioned according to the distance to \(|\psi\rangle\). It is known that if stochastic one-qubit operations are used, entanglement of three [12] and four [13] qubits fall into respectively two and nine different classes. Our classification according to the number of CNOTs is different, although there are some relations. Our results generalize to other universal two-qubit gates, in particular to the iSWAP gate which has been shown to be implementable for superconducting qubits [14].

We consider pure states belonging to the 2^n-dimensional Hilbert space \(\mathbb{C}^{2^n}\). The space of normalized quantum states is the sphere \(S^{2^n+1-1}/U(2)^n\) of states nonequivalent under \(U(2)\). As the cost of one-qubit gates is negligible, we are interested only in equivalence classes of states modulo local unitary transformations (LU). We thus consider the sets \(\mathcal{E}_n = S^{2^n+1-1}/U(2)^n\) of states nonequivalent under LU. In the case of two and three qubits the dimension of \(\mathcal{E}_2\) and \(\mathcal{E}_3\) was determined in [12, 13] and their topology has been described in [17]. Throughout the paper we will make use of the one-qubit LU operations \(R^{(k)}_j (\xi) = \exp(-i\xi \sigma_j^{(k)})\) where the \(\sigma_j^{(k)}\) are the Pauli matrices acting on qubit \(k\). In particular, the operation \(R^{(k)}_y (\xi)\) corresponds to a rotation of the qubit \(\cos(\varphi)|0\rangle + \sin(\varphi)|1\rangle \mapsto \cos(\varphi + \xi)|0\rangle + \sin(\varphi + \xi)|1\rangle\).

Two-qubit states. Let us first consider the two-qubit case. It has been shown in [14] that one can transform an arbitrary two-qubit state \(|\psi\rangle\) to \(|00\rangle\) by using only one CNOT. Here we prove that the same holds for two general two-qubit states \(|\psi\rangle\) and \(|\psi'\rangle\).

Proof: Since \(\mathcal{E}_2\) is homeomorphic to \([0, 1]\), only one
parameter (e.g., one Schmidt coefficient) characterizes a state up to LU. More precisely, by LU each two-qubit state can be brought to the canonical form $|\psi\rangle = \cos \varphi |00\rangle + \sin \varphi |11\rangle$, which is just Schmidt decomposition. We want to transform state $|\psi\rangle$ with parameter $\varphi$ to state $|\psi'\rangle$ with parameter $\varphi'$. When $\varphi' \neq \varphi$, we need at least one CNOT. It turns out that one CNOT is in fact sufficient, as can be easily seen by checking that the relation $R_{\psi}^{(1)}(-\varphi)\text{CNOT}_{12}R_{\psi}^{(2)}(\varphi)|\psi\rangle = |\psi'\rangle$ holds (by convention, qubit 1 is the leftmost one).

In contrast, one needs three CNOTs in general to construct a specific two-qubit unitary transformation $[3]$. Transforming one state to another is thus clearly easier.

We now turn to the three-qubit case.

**Classification with respect to $|000\rangle$.** We start with the case where we want to prepare a state $|\psi\rangle$ from $|000\rangle$. The distance (in number of CNOTs) from $|000\rangle$ to $|\psi\rangle$ is a criterion for the difficulty to prepare $|\psi\rangle$. We will show that this distance partitions the Hilbert space into four classes, and that any state can be prepared from $|000\rangle$ using three CNOT gates or less. We will examine each of these four classes in turn.

**Class 0:** One needs zero CNOT gates to transform $|\psi\rangle$ to $|000\rangle$ iff the state is of the product form $|\psi\rangle = |\alpha\beta\gamma\rangle$, where $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ are normalized single qubit states (this is trivial, since only LU are used).

**Class 1:** One needs one CNOT iff the state is of the form $|\psi\rangle = |\alpha\rangle_1|\chi\rangle_{23}$ (i.e., it is bi-separable), where $|\chi\rangle_{23}$ is an arbitrary entangled state of the last two qubits $[18]$.

**Proof:** By LU $|\psi\rangle$ can be transformed into canonical form $|\psi\rangle \overset{LU}{=} |0\rangle(\cos \varphi |00\rangle + \sin \varphi |11\rangle)$. Applying CNOT 23 to this canonical form we obtain $|0\rangle(\cos \varphi |00\rangle + \sin \varphi |10\rangle)$, i.e., state $|0\rangle(\cos \varphi |0\rangle + \sin \varphi |1\rangle)|0\rangle$ which is in class 0.

We can therefore reach $|000\rangle$ in a single CNOT step. Conversely, applying one CNOT gate on a state from class 0 the state reached is bi-separable and therefore all states that need 1 step to get from $|000\rangle$ are of the above form.

In their canonical form states from class 1 can be parametrized by a single real parameter $\varphi$.

**Class 2:** One needs two CNOT gates iff the state is of the form $|\psi\rangle = \cos \varphi |\alpha\beta\gamma\rangle + \sin \varphi |\alpha\perp\beta'\gamma'\rangle$, with $\langle\alpha|\alpha\perp\rangle = 0$, $|\langle\beta|\beta'\rangle| < 1$ and $|\langle\gamma|\gamma'\rangle| < 1$ (if $|\langle\beta|\beta'\rangle|$ or $|\langle\gamma|\gamma'\rangle|$ are equal to 1 then $|\psi\rangle$ belongs to class 1).

**Proof:** We first bring the state by LU to the canonical form $|\psi\rangle \overset{LU}{=} \cos \varphi |00\rangle + \sin \varphi |1\beta\gamma\rangle$. If the phases are absorbed into the definition of local bases, $|\gamma\rangle$ can be written as $\cos \xi |0\rangle + \sin \xi |1\rangle$. The rotation $R_{\psi}^{(3)} \left( \frac{\pi}{2} - \frac{\xi}{2} \right)$ followed by a CNOT$_{13}$ yields a state $(\cos \varphi |00\rangle + \sin \varphi |1\beta\rangle)|\gamma\rangle$, which is a state of class 1 from which we can reach state $|000\rangle$ in a single step.

To prove the converse, we have to show that by using two CNOT gates one can reach only states of the form $|\psi\rangle = \cos \varphi |\alpha\beta\gamma\rangle + \sin \varphi |\alpha\perp\beta'\gamma'\rangle$, or states in class 0 or class 1. Starting from class 0, we are in class 1 after one step. Any class 1 state can be written as $|\alpha\rangle(\cos \varphi |0\rangle + e^{i\xi} \sin \varphi |1\rangle)$. Applying CNOT$_{23}$ or CNOT$_{32}$ we get a state in class 0 or class 1. Applying CNOT$_{21}$ on the other hand we get $\cos \varphi |0\rangle + e^{i\xi} \sin \varphi |1\rangle$, where $|\varphi\rangle = \sigma_x |\alpha\rangle$, which is indeed of the canonical form of class 2 states. Last possibility is applying CNOT$_{12}$. In this case it is better to write our state in the basis $(|\pm\rangle = (|0\rangle \pm |1\rangle)/\sqrt{2}$ for the second qubit. That is, any class 1 state can be written as $|\alpha\rangle(\cos \varphi - \gamma) + e^{i\xi} \sin \varphi |\gamma\rangle$.

Writing $|\alpha\rangle = \cos \varphi |0\rangle + e^{i\xi} \sin \varphi |1\rangle$, then we get after applying CNOT$_{12}$ state $|\alpha\rangle(\cos \varphi |0\rangle - e^{i\xi} \sin \varphi |1\rangle)|\gamma\rangle + \sin \varphi e^{i\xi}(\cos \varphi |0\rangle + e^{i\xi} \sin \varphi |1\rangle)|\gamma\rangle$, which is again of the canonical form expected. For CNOT$_{13}$ or CNOT$_{31}$ the argument is similar.

One needs 3 real parameters to describe states of class 2 in their canonical form. Note that class 2 states constitute a subset of GHZ type states which are of (unnormalized) form $|\alpha\beta\gamma\rangle + |\alpha'\beta'\gamma\rangle$ $[12]$.

**Class 3:** One needs three CNOT gates iff a state is not in class 0, 1 or 2.

**Proof:** States not in the previous classes are of two types: (i) W-like states (according to the classification in $[12]$) for which the range of the reduced density matrix of qubits 2 and 3 contains only one product state. Such states are of the (unnormalized) form $|\psi\rangle = |\alpha\beta\gamma\rangle + |\alpha'\chi\rangle_{23}$, where $|\chi\rangle_{23}$ is entangled and orthogonal to $|\beta\gamma\rangle$. Under LU they can be written in the following canonical form $[12]$

$$|\psi\rangle \overset{LU}{=} \cos \varphi |000\rangle + \sin \varphi |01\rangle,$$

with $|\varphi\rangle = \cos \xi |0\rangle + \sin \xi |1\rangle$ and, (ii) GHZ-like states with the canonical form

$$|\psi\rangle \overset{LU}{=} a|000\rangle + e^{i\xi} b|\alpha\beta\gamma\rangle,$$

where $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$ are real single qubit states parametrized by one parameter each and $a, b$ are real parameters, one of which is fixed by normalization $[19]$.

To exclude class 2 states we must demand that none of $|\alpha\rangle$, $|\beta\rangle$ and $|\gamma\rangle$ be equal to $|1\rangle$. To exclude class 1 and 0 states in $[1, 2]$ $\rho_{23}$ must be of rank 2. W-like states $[1]$ require 3 parameters. GHZ-like $[2]$ states need 5, and thus are the generic states.

First we show that by using single CNOT one can transform class 3 states to class 2. For W-like states $[1]$ we just have to apply CNOT$_{23}$ to the canonical form $[1]$ and we immediately get $\cos \varphi |000\rangle + \sin \varphi |01\rangle |\alpha\beta\gamma\rangle$ which is of class 2 (states on the third qubit are orthogonal). For GHZ-like states $[2]$ it is a bit more work. Note that GHZ-type states can be, by rearranging terms and after LU, written as $\cos \varphi |000\rangle + \sin \varphi |1\rangle |\chi\rangle_{23}$ (expanding $|0\rangle$ on the first qubit in $[2]$ into $|\alpha\rangle$ and $|\alpha\perp\rangle$ and adding $|\alpha\rangle$ part to the second term), where $|\chi\rangle_{23}$ can in turn be expanded as $|\chi\rangle_{23} = \cos \varphi |0\delta\rangle + \sin \varphi |1\delta\rangle$ with $|\langle\delta|\delta\rangle| < 1$ (otherwise state would be in class 2). Finally, rotating third qubit brings the state to
The results above show that the number of CNOTs in the canonical form (3) are unique. λ where the six parameters form (22) has the same invariants (i.e., is the same up to distance 1 from the GHZ state χ). Converstely, if a state |ψ⟩ is in canonical form (1), one can check that the state CNOT23 RY(1) 3 (θ1) |ψ⟩, with parameters respectively θ1, φ2, and φ3. Normalization imposes that a2 + b2 + 2ab cos ξ cos φ1 cos φ2 cos φ3 = 1. One can check that the state CNOT12 RY(1) 1 (θ1) RY(2) 2 (θ2) |ψ⟩, with parameters of the rotations given by

\[
\begin{align*}
\tan 2\theta_1 &= \frac{(b^2 - a^2) \cos 2\varphi_1 - a^2 (a^2 - 1 - 2b^2 \cos^2 \varphi_1 \cos 2\varphi_2 + 2b^4 \cos^2 \varphi_2 \sin^2 (2\varphi_1) \sin^2 \varphi_3)}{b^2 \sin (2\varphi_1) \left(1 - a^2 - b^2 + 2a^2 \cos^2 \varphi_2 (1 - a^2 \sin^2 \varphi_3 + b^2 \cos(2\varphi_2) \sin^2 \varphi_3) \right)} \\
\tan 2\theta_2 &= -\frac{b^2 \sin (2\varphi_1 + 2\theta_1) \sin 2\varphi_2 + 2ab \cos \xi \sin (\varphi_1 + 2\theta_1) \sin \varphi_2 \cos \varphi_3}{a^2 \sin 2\theta_1 + b^2 \sin (2\varphi_1 + 2\theta_1) \cos 2\varphi_2 + 2ab \cos \xi \sin (\varphi_1 + 2\theta_1) \cos \varphi_2 \cos \varphi_3} \\
\tan 2\varphi &= -\frac{2ab \sin \xi \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 (a^2 \sin 2\theta_1 - b^2 \sin (2\varphi_1 + 2\theta_1))}{2a \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 (a^2 \sin 2\theta_1 + b^2 \sin (2\varphi_1 + 2\theta_1))}
\end{align*}
\]

verifies I1 = 1/2. The results above show that the number of CNOTs
needed to transform a state to another state is much less
than the number to produce all unitary transformations. 
Indeed, according to [10], one needs at least 14 CNOT
 gates to produce any three-qubit unitary transformation.
Our procedure is explicit, and selects a specific unitary
transformation leading from one state to the other using
less CNOTs than a general unitary transformation.

Let us now discuss the applicability of these results to
physical systems. In an experimental context, our re-
sults can be used to construct any desired state from the
initial state which is easiest to produce with a given sys-
tem. In some experimental set-ups, two-qubit gates are
built from a nearest neighbor interaction (for example
in [5, 6]). In this case, the common procedure is to use
additional SWAP gates to transfer the states of two dis-
tant qubits to nearest neighbors before performing the
CNOTs. However, in our case, due to the symmetry of
GHZ state, one can go from any state to the GHZ state
in two CNOTs without the need of any quantum SWAP.
Thus even if only nearest-neighbors CNOTs are available
for three qubits on a line, still only 4 CNOTs are enough
to go from any state to any other state. If one starts
from |000⟩ and one allows for relabeling of qubits in the
final state, 3 CNOTs are still enough to go to any state,
except for the GHZ-type class 3 states, Eq. [2], which
need an additional CNOT in this architecture.

Any two-qubit gate can be expressed in terms of
CNOTs and one-qubit gates. Thus our result will im-
ply a bound in the number of two-qubit gates needed to
go from one three-qubit state to another, for any other
choice of universal two-qubit gate. We note that another
popular two-qubit gate is the iSWAP which is natural
for implementations corresponding to a XY-interaction.
As the iSWAP can be expressed in terms of one CNOT
and one SWAP gate plus one-qubit gates [23], our re-
sults apply directly to this particular gate provided the
SWAP can be made classically: the number of iSWAPs
needed to transform three qubits is then the same as for
CNOTs. This in particular arises when the physical im-
plementation allows for a coupling between any pair of
qubits, as swapping two qubits is equivalent to relabeling
the qubits for all subsequent gates by interchanging the
role of the qubits. An important example is the case of
superconducting qubits coupled to each other via cavity
bus [14], one of the most promising recent developments,
where the resonance can be tuned to couple any pair.

In conclusion, we have shown that one needs only
three CNOTs plus additional one-qubit gates to trans-
form |000⟩ to any pure three-qubit states. If one starts
from the GHZ state, only two CNOTs are enough, and
thus one needs only four CNOTs plus additional one-
qubit gates to transform any initial pure three-qubit state
to any other pure three-qubit states. An interesting open
question is to find out whether four is the maximal dis-
tance between two three-qubit states (it should be at
least three since |000⟩ is at distance 3 from class 3 states).
It would be also interesting to know how these results
translate to mixed states, or to pure states using SLOCC
instead of LU. At last, generalizations to higher numbers
of qubits may pave the way to better optimization of
quantum algorithms, which are usually described as unit-
ary operators but are sometimes just transformations of
a given state into another one.

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the calculations, so that, e.g., state |α⟩1|χ⟩23 also
represents |χ⟩2|α⟩13 and |α⟩2|χ⟩13. As we deal with distances from
symmetric states such as |000⟩ and GHZ, this amounts
to relabeling the gates, without any loss of generality.
[19] Indeed, the rank of the reduced density matrix ρ23 ob-
tained by tracing out the first qubit is at most two. If it
is two, then the range of ρ23 contains at least one prod-
uct vector. If it contains only one, one has class 3(i)
states, otherwise one has class 3(ii) or class 2 states.
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