

Optimal number of controlled-NOT gates to generate a three-qubit state

Marko Žnidarič,¹ Olivier Giraud,² and Bertrand Georgeot²

¹*Department of Physics, Faculty of Mathematics and Physics, University of Ljubljana, SI-1000 Ljubljana, Slovenia*

²*Laboratoire de Physique Théorique, Université de Toulouse, UPS, CNRS, 31062 Toulouse, France*

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The number of two-qubit gates required to deterministically transform 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 Greenberger-Horne-Zeilinger 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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I. INTRODUCTION

Quantum information and computation (see, e.g., Ref. [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 than 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, the results of Ref. [11] show that one CNOT is enough to go from any given pure state to any other. Here we give an explicit algorithm achieving that. 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 Greenberger-Horne-Zeilinger (GHZ) state $(|000\rangle + |111\rangle)/\sqrt{2}$. 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 $S^{2^{n+1}-1}$. As the cost of one-qubit gates is negligible, we are interested only in equivalence classes of states modulo local unitary (LU) transformations. We thus consider the sets $\mathcal{E}_n = S^{2^{n+1}-1}/U(2)^n$ of states nonequivalent under LU transformations. In the case of two and three qubits the dimension of \mathcal{E}_2 and \mathcal{E}_3 was determined in Refs. [15,16] and their topology has been described in Ref. [17]. Throughout the paper we will make use of the one-qubit LU operations $R_j^{(k)}(\xi) = \exp(-i\xi\sigma_j^{(k)})$ where the $\sigma_j^{(k)}$ are the Pauli matrices acting on qubit k . In particular, the operation $R_y^{(k)}(\xi)$ corresponds to a rotation of the qubit $\cos(\varphi)|0\rangle + \sin(\varphi)|1\rangle \mapsto \cos(\varphi + \xi)|0\rangle + \sin(\varphi + \xi)|1\rangle$.

II. TWO-QUBIT STATES

We first give an explicit algorithm that transforms a general two-qubit state $|\psi\rangle$ into another state $|\psi'\rangle$ using only one CNOT.

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 φ to state $|\psi'\rangle$ with parameter φ' . 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 $R_y^{(1)}(-\varphi)\text{CNOT}_{12}R_y^{(1)}(\varphi)|\psi\rangle=|\psi'\rangle$ holds (by convention, qubit 1 is the leftmost one). ■

In contrast, one needs three CNOT s in general to construct a specific two-qubit unitary transformation [9]. Transforming one state to another is thus clearly easier.

III. THREE-QUBIT STATES

We now turn to the three-qubit case. In the following, we investigate the minimal number of CNOT gates required to generate any given three-qubit state from two different choices of initial state.

A. 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 $|000\rangle$ if and only if 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 if and only if the state is of the form $|\psi\rangle=|\alpha\rangle_1|\chi\rangle_{23}$ (i.e., it is biseparable), 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 LU $|\psi\rangle=|0\rangle(\cos\varphi|00\rangle+\sin\varphi|11\rangle)$. 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 biseparable 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 φ .

Class 2. One needs two CNOT gates if and only if 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 LU $|\psi\rangle=\cos\varphi|000\rangle+\sin\varphi|1\beta\gamma\rangle$. 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 $R_y^{(3)}(\frac{\pi}{4}-\frac{\xi}{2})$ 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 $|\alpha\rangle(\cos\varphi|0\rangle+e^{i\xi}\sin\varphi|1\rangle)|\gamma'\rangle$. 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

$\cos\varphi|\alpha0\rangle+e^{i\xi}\sin\varphi|\alpha1\rangle|\gamma'\rangle$, where $|\alpha\rangle=\sigma_x|\alpha\rangle$, 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 $|\alpha\rangle(\cos\varphi|-\rangle+e^{i\xi}\sin\varphi|+\rangle)|\gamma'\rangle$. Writing $|\alpha\rangle=\cos\varphi'|0\rangle+e^{i\xi'}\sin\varphi'|1\rangle$, we then get after applying the CNOT_{12} state $\cos\varphi(\cos\varphi'|0\rangle-e^{i\xi'}\sin\varphi'|1\rangle)|-\rangle+\sin\varphi e^{i\xi}(\cos\varphi'|0\rangle+e^{i\xi'}\sin\varphi'|1\rangle)|+\rangle$, which is again of the canonical form expected. For CNOT_{13} or CNOT_{31} the argument is similar. ■

One needs three 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 if and only if 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 defined by the property that the range of the reduced density matrix of qubits 2 and 3 contains only one product state. Such states are of the (un-normalized) form $|\psi\rangle=|\alpha\beta\gamma\rangle+|\alpha'\rangle|\chi\rangle_{23}$, where $|\chi\rangle_{23}$ is entangled and orthogonal to $|\beta\gamma\rangle$. Under LU they can be written in the following canonical form [12]

$$\text{LU} \quad |\psi\rangle=\cos\varphi|000\rangle+\sin\varphi|\alpha\rangle(\cos\varphi'|10\rangle+\sin\varphi'|01\rangle), \quad (1)$$

with $|\alpha\rangle=\cos\xi|0\rangle+\sin\xi|1\rangle$ and (ii) *GHZ-like* states [19,20] with the canonical form

$$\text{LU} \quad |\psi\rangle=a|000\rangle+e^{i\xi}b|\alpha\beta\gamma\rangle, \quad (2)$$

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. 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 Eqs. (1) and (2) ρ_{23} must be of rank 2. *W-like* states (1) require three 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 $\cos\varphi|000\rangle+\sin\varphi|\alpha\rangle(\cos\varphi'|1\rangle+\sin\varphi'|0\rangle)|1\rangle$ 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 Eq. (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 $\cos\varphi|00\gamma'\rangle+\sin\varphi|1\rangle(\cos\varphi'|00\rangle+e^{i\xi'}\sin\varphi'|1\gamma'\rangle)$ with real $|\gamma'\rangle=\cos g'|0\rangle+\sin g'|1\rangle$. After application of the rotation $R_y^{(3)}(\frac{\pi}{4}-\frac{g'}{2})$ followed by CNOT_{23} we arrive at $\cos\varphi|00\tilde{\gamma}'\rangle+\sin\varphi|1\rangle(\cos\varphi'|0\rangle+e^{i\xi'}\sin\varphi'|1\rangle)|\tilde{\gamma}'\rangle$ which is of class 2. Since the canonical forms of classes 0, 1, 2, and 3 span the whole Hilbert space and since the forms of classes 0, 1 and 2 are the only ones that can be reached in 2 steps, it immediately follows that the states of canonical

forms (1) and (2) require exactly three steps. ■

Thus any state is at a distance less than or equal to 3 from $|000\rangle$.

B. Classification with respect to GHZ state

Let us now examine the distance to the GHZ state $|\text{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$. It turns out that any state is at a distance less than or equal to 2 from GHZ. We use the fact that any state in \mathcal{E}_3 can be characterized by a set of six polynomial invariants [21,22]. Following Ref. [22], we denote the first three invariants by $I_i = \text{tr } \rho_i^2$, $1 \leq i \leq 3$, where ρ_i is the reduced density matrix of the i th qubit. Any three-qubit state is equivalent under LU to its canonical form [22]

$$\lambda_0|000\rangle + \lambda_1 e^{i\phi}|100\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle, \quad (3)$$

where the six parameters $\lambda_0, \dots, \lambda_4, \phi$ label the state in \mathcal{E}_3 and $\sum \lambda_i^2 = 1$. If we take $0 \leq \phi \leq \pi$ the parameters in the canonical form (3) are unique.

Class 0. States at distance 0 from GHZ are states whose canonical form (3) is GHZ (this is trivial).

Class 1. States at distance 1 from GHZ are states whose canonical form (3) is (up to relabeling)

$$\frac{1}{\sqrt{2}}|000\rangle + \lambda_2|101\rangle + \lambda_3|110\rangle + \lambda_4|111\rangle \quad (4)$$

(with $\lambda_4 \neq 1/\sqrt{2}$), i.e., states with $I_1 = \frac{1}{2}$.

Proof. It is straightforward to check that the state (4) has the same invariants (i.e., is the same up to LU) as $\text{CNOT}_{23} R_y^{(2)}(\theta_2) R_y^{(3)}(\theta_3) |\text{GHZ}\rangle$ with $\theta_2 = \frac{1}{2} \arcsin(\lambda_2 \sqrt{2})$ and $\theta_3 = \frac{1}{2} \arccos(\lambda_3 \sqrt{2})$, and thus is at distance 1 from GHZ. Conversely, if a state $|\psi\rangle$ is at distance 1 from GHZ, then one of its invariants I_1, I_2, I_3 has to be the same as for GHZ. Since GHZ is symmetric under permutation of the qubits, one can consider that the CNOT gate applied is CNOT_{23} (up to relabeling of the qubits before applying the CNOT). In this case the

invariant $I_1 = \frac{1}{2}$ is conserved. The reduced density matrix of the first qubit of $|\psi\rangle$ therefore verifies $\text{tr } \rho_1^2 = \frac{1}{2}$ which in turn (since it is a 2×2 density matrix) implies that $\rho_1 = \frac{1}{2} \mathbb{1}$. All states with this property can be written as $|\psi\rangle = \frac{1}{\sqrt{2}}|0\rangle|\chi\rangle + \frac{1}{\sqrt{2}}|1\rangle|\chi_\perp\rangle$, with $\langle\chi|\chi_\perp\rangle = 0$. The canonical form of such states is precisely (4). ■

Class 2. All other states are at distance 2 from GHZ.

Proof. We show that all other states are at distance 1 from states of canonical form (4). States of canonical form (4) are characterized by $I_1 = \frac{1}{2}$. Therefore we have to prove that any state $|\psi\rangle$ not in class 0 or 1 can be transformed to a state verifying $I_1 = \frac{1}{2}$ with only one CNOT gate. The reduced density matrix of the first qubit is a 2×2 matrix $\rho_1 = \begin{pmatrix} A & B \\ B^* & 1-A \end{pmatrix}$. The first invariant is thus given by $I_1 = A^2 + (1-A)^2 + 2|B|^2$. It is equal to $\frac{1}{2}$ if and only if $A = \frac{1}{2}$ and $B = 0$, which (since B is complex) yields three equations. One-parameter rotations of the qubits before applying CNOT yield free parameters. It turns out that a solution to the three equations always exists. Indeed, the state $|\psi\rangle$ can be reduced either to the canonical form (1) or to the canonical form (2). If $|\psi\rangle$ is in canonical form (1), one can check that the state $\text{CNOT}_{12} R_y^{(1)}(\theta_1) R_y^{(2)}(\theta_2) |\psi\rangle$, with

$$\tan 2\theta_1 = \frac{\cot^2 \varphi + \cos 2\xi}{\sin 2\xi},$$

$$\tan 2\theta_2 = \frac{\sin(\xi + 2\theta_1) \cos \varphi' \sin 2\varphi}{\sin(2\xi + 2\theta_1) \cos 2\varphi' \sin^2 \varphi - \cos^2 \varphi \sin 2\theta_1} \quad (5)$$

is such that $I_1 = \frac{1}{2}$. Let us now suppose that $|\psi\rangle$ is in canonical form (2). The one-qubit states $|\alpha\rangle, |\beta\rangle, |\gamma\rangle$ can be written in the form $\cos \varphi|0\rangle + \sin \varphi|1\rangle$ with parameters, respectively, φ_1, φ_2 , and φ_3 . Normalization imposes that $a^2 + b^2 + 2ab \cos \xi \cos \varphi_1 \cos \varphi_2 \cos \varphi_3 = 1$. One can check that the state $\text{CNOT}_{12} R_x^{(1)}(\chi) R_y^{(1)}(\theta_1) R_y^{(2)}(\theta_2) |\psi\rangle$, with parameters of the rotations given by

$$\begin{aligned} \tan 2\theta_1 &= \frac{(b^2 - b^4) \cos 2\varphi_1 - a^2(a^2 - 1 - 2b^2 \cos^2 \varphi_1 \cos 2\varphi_2 + 2b^4 \cos^2 \varphi_2 \sin^2(2\varphi_1) \sin^2 \varphi_3)}{b^2 \sin(2\varphi_1) \{1 - a^2 - b^2 + 2a^2 \cos^2 \varphi_2 [1 - a^2 \sin^2 \varphi_3 + b^2 \cos(2\varphi_1) \sin^2 \varphi_3]\}}, \\ \tan 2\theta_2 &= - \frac{b^2 \sin(2\varphi_1 + 2\theta_1) \sin 2\varphi_2 + 2ab \cos \xi \sin(\varphi_1 + 2\theta_1) \sin \varphi_2 \cos \varphi_3}{a^2 \sin 2\theta_1 + b^2 \sin(2\varphi_1 + 2\theta_1) \cos 2\varphi_2 + 2ab \cos \xi \sin(\varphi_1 + 2\theta_1) \cos \varphi_2 \cos \varphi_3}, \\ \tan 2\chi &= - \frac{2ab \sin \xi \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 [a^2 \sin 2\theta_1 - b^2 \sin(2\varphi_1 + 2\theta_1)]}{2a \sin \varphi_1 \sin \varphi_2 [2ab^2 \cos \varphi_1 \cos \varphi_2 + b(a^2 + b^2) \cos \xi \cos \varphi_3]}, \end{aligned} \quad (6)$$

verifies $I_1 = \frac{1}{2}$. ■

IV. DISCUSSION

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 Ref. [10], one needs at least 14 CNOT gates to produce any three-qubit unitary transformation. We also note that the best available algorithm actually does not saturate the bound, needing 20 CNOTs [10]. Our procedure improves

previous algorithms for pure states which needed 10 CNOTs [10]. It 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 results can be used to construct any desired state from the initial state which is easiest to produce with a given system. In some experimental setups, two-qubit gates are built from a nearest neighbor interaction (for example, in Refs. [5,6]). In this case, the common procedure is to use additional SWAP gates to transfer the states of two distant 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 four CNOTs are enough to go from any state to any other state. If one starts from $|000\rangle$ and one allows for relabeling of qubits in the final state, three 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 imply 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 ($|00\rangle \rightarrow |00\rangle$, $|01\rangle \rightarrow i|10\rangle$, $|10\rangle \rightarrow i|01\rangle$, $|11\rangle \rightarrow |11\rangle$) 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 results 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 implementation 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.

V. CONCLUSION

In conclusion, we have shown that one needs only three CNOTs plus additional one-qubit gates to transform $|000\rangle$ 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 distance between two three-qubit states (it should be at least three since $|000\rangle$ 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 stochastic local operations and classical communication 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 unitary operators but are sometimes just transformations of a given state into another one.

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without any loss of generality.

- [19] If the rank of the reduced density matrix ρ_{23} obtained by tracing out the first qubit is two, then the range of ρ_{23} contains at least one product vector [20]. If it contains only one, we call the state *W*-like (1), otherwise if it is not in class 2 we call it *GHZ*-like (2).

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