# Multipartite entanglement in quantum algorithms

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We investigate the entanglement features of the quantum states employed in quantum algorithms. In particular, we analyze the multipartite entanglement properties in the Deutsch-Jozsa, Grover, and Simon algorithms. Our results show that for these algorithms most instances involve multipartite entanglement.

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## I. INTRODUCTION

Entanglement is a major resource in quantum information processing. However, its role in achieving the quantum computational speedup in the currently known quantum algorithms is not yet completely clear and has been a highly debated question since the advent of quantum computation. In particular, the role of genuine *multipartite* entanglement has not been elucidated thoroughly. It was shown that in Shor's algorithm multipartite entanglement is needed to achieve exponential computational speedup with quantum resources [1]. In this work we analyze other known quantum algorithms, namely, those of Deutsch-Jozsa, Grover, and Simon, and assess the multipartite entanglement properties of the pure quantum states employed.

In the Deutsch-Jozsa [2] and Grover [3] algorithms, following the formulation given in [4], the $n$-qubit states that occur are of the form

$$|\psi_f\rangle \equiv \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} (-1)^{f(x)} |x\rangle \ , \tag{1}$$

where $|x\rangle$ represent the computational basis states of $n$ qubits and $f(x)$ is the $\{0,1\}^n \rightarrow \{0,1\}$ Boolean function that needs to be evaluated. Notice that $(-1)^{f(x)} = \pm 1$ is just a real phase factor.

The above states are achieved by starting from the equally weighted superposition of all possible $2^n$ states in the computational basis, namely, the state

$$|\psi_0\rangle \equiv \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} |x\rangle \ , \tag{2}$$

and then applying a unitary transformation $U_f$, which involves an additional qubit (a target qubit) and acts as follows:

$$U_f |x\rangle |y\rangle = |x\rangle |f(x) \oplus y\rangle \ . \tag{3}$$

In the above expression $|y\rangle$ is the state of the target qubit and $\oplus$ denotes addition modulo 2. The target qubit is initially prepared in the state $|-\rangle \equiv (|0\rangle - |1\rangle)/\sqrt{2}$. In this way the target state is left unchanged by the action of $U_f$ and the state of the $n$-qubit register takes the form (1). The above states will be referred to as multiqubit "real equally weighted states" $|\psi_f\rangle$.

The paper is organized as follows. In Sec. II we will concentrate on the Deutsch-Jozsa algorithm and discuss the entanglement properties of the corresponding multiqubit real equally weighted states. In Sec. III we will consider the Grover algorithm and analyze the corresponding states for different values of the number of solutions. In Sec. IV we will study the case of the Simon algorithm, and we will summarize the results in Sec. V.

## II. THE DEUTSCH-JOZSA ALGORITHM

In the Deutsch-Jozsa algorithm, the function $f$ to be evaluated is promised to be either constant or balanced (balanced means that it takes output 0 for half of the inputs and output 1 for the others). The state (1), where a minus sign is present in front of half of the computational basis states and will therefore be called a balanced state, can be either separable or entangled. The state (1) is separable if and only if it can be expressed in the form

$$|\psi_{\rm sep}\rangle \equiv \frac{1}{\sqrt{2^n}} \sum_{x=0}^{2^n-1} (-1)^{ax} |x\rangle \ , \tag{4}$$

where $a$ is an $n$-bit string and $ax \equiv a_1 x_1 \oplus a_2 x_2 \oplus \cdots a_n x_n$. Therefore, apart from global phase factors, the number of distinct separable states of the form (1) is $2^n$. If the function $f$ is constant the state $|\psi_f\rangle$ is clearly separable, and apart from a global phase factor, it is the state $|\psi_0\rangle$ [in this case the string $a$ in the form (4) has all bits 0]. Notice that the above state in Eq. (4) corresponds exactly to the state computed in the Bernstein-Vazirani problem [5], where the function is promised to be of the form $f_a(x) = ax$ and the question is to find $a$. Therefore, for the Bernstein-Vazirani problem, which can be solved as the Deutsch-Jozsa problem restricted to the particular class of functions of the form $f_a$, the qubits involved are never entangled. This has already been observed in [6].

In general, if the function $f$ is balanced, the state (1) can then be either separable or entangled. We will now evaluate the number of separable vs entangled states. The number of possible balanced functions is given by $N_{\rm bal} = B(2^n, 2^{n-1})$, where $B$ denotes the binomial coefficient. The number of balanced functions corresponding to separable states, which are then necessarily of the form (4), is $N_{\rm bal,sep} = 2(2^n - 1)$. This value is obtained by noticing that two different balanced functions correspond to each $a$ (they would correspond to states $|\psi_s\rangle$ and $-|\psi_s\rangle$, which differ just in a global phase factor), while the case of vanishing $a$ does not correspond to a balanced function and therefore must be subtracted. The fraction of balanced functions that involve separable states with respect to the total is therefore given by $N_{\rm bal,sep}/N_{\rm bal} = 2(2^n-1)(2^{n-1}!)^2/2^n!$. Using the Stirling approximation, i.e., $\lim_{x\to\infty} x! \approx \sqrt{2\pi x}x^x e^{-x}$, we arrive at the asymptotic limit $\lim_{n\to\infty} N_{\rm bal,sep}/N_{\rm bal} \approx \sqrt{2\pi}(2^n-1)2^{\frac{n}{2}}/2^{2^n}$. Thus, for large numbers of qubits the fraction of separable balanced states becomes doubly exponentially small, i.e., for most balanced functions the Deutsch-Jozsa algorithm employs entangled states.

In the following we will denote by $S_q$ the set of pure $q$-separable states, i.e., states that can be written as tensor products of pure states of $q$ subsystems [7]. So far we have evaluated the fraction of fully separable states (i.e., $\in S_n$). We can also evaluate the fraction of states that are not fully separable but contain entanglement only between two qubits (i.e., $\in S_{n-1}\backslash S_n$). Actually, these kinds of states are of the form $|\psi_{\rm sep,n-2}\rangle \otimes |\psi_{\rm ent,2}\rangle$. There are $2(2^{n-2}-1)*8$ distinct balanced functions that correspond to states of this form: the factor $2(2^{n-2}-1)$ is the number of balanced functions corresponding to fully separable states of $n-2$ qubits, while 8 is the number of entangled real equally weighted states of two qubits (four states with just a minus sign in the superposition and four states with three minus signs). States of this type can occur for $B(n,2)$ different partitions of the $n$ qubits; therefore, the total number of balanced functions corresponding to states in $S_{n-1}\backslash S_n$ is $2(2^{n-2}-1)*8*B(n,2)$. By taking the limit of large $n$ we can see that the fraction of these functions over the total number $N_{\rm bal}$ is still exponentially small.

Rather than evaluating all possible classes of states we will answer the question of whether most states in the Deutsch-Jozsa algorithm (in the limit $n\to\infty$) are genuinely multipartite entangled. To this end, we count the number of biseparable balanced states, i.e., states in $S_2$ corresponding to balanced functions that are of the form

$$|\psi_{\rm bisep}\rangle = |\psi_k\rangle \otimes |\psi_{n-k}\rangle, \tag{5}$$

and their fraction within all balanced states. Here, it does not matter whether the constituting states are entangled or separable, because any pure state that cannot be written in a biseparable form is fully entangled. Before counting the number of biseparable balanced states, we will establish when a biseparable state is balanced.

**Lemma:** For a pure real equally weighted state of $n$ qubits that is $q$-separable, i.e.,

$$|\psi_{q-{\rm sep}}\rangle = |\psi_{k_1}\rangle \otimes |\psi_{k_2}\rangle \otimes \cdots |\psi_{k_p}\rangle, \text{ with } \sum_{i=1}^{q} k_i = n; \qquad q>1, \tag{6}$$

where each $|\psi_{k_i}\rangle$ is real equally weighted, the state $|\psi_{q-{\rm sep}}\rangle$ is *balanced* if and only if at least one $|\psi_{k_i}\rangle$ is balanced.

*Proof:* Denote by $N^{(k)}_{+(-)}$ the number of plus (minus) signs of a real equally weighted state with $k$ qubits.

"$\Rightarrow$": For a balanced $n$-qubit state we have $N_+^{(n)} = N_-^{(n)}$. For each partition with $k_i$ qubits in one subsystem, and $n-k_i$ in the other subsystem, we thus have $N_+^{(k_i)}\cdot N_+^{(n-k_i)} + N_-^{(k_i)}\cdot N_-^{(n-k_i)} = N_+^{(k_i)}\cdot N_-^{(n-k_i)} + N_-^{(k_i)}\cdot N_+^{(n-k_i)}$ or $N_+^{(n-k_i)}(N_-^{(k_i)} - N_+^{(k_i)}) = N_-^{(n-k_i)}(N_-^{(k_i)} - N_+^{(k_i)})$. The solution of this equation is either $N_+^{(n-k_i)} = N_-^{(n-k_i)}$ or $N_+^{(k_i)} = N_-^{(k_i)}$, i.e., at least one of the two subsystems is in a balanced state. This argument holds for all possible partitions.

"$\Leftarrow$": Assume without loss of generality that $|\psi_{k_1}\rangle$ is balanced, i.e., $N_+^{(k_1)} = N_-^{(k_1)}$. The number of plus signs in the $n$-qubit state is $N_+^{(n)} = N_+^{(k_1)}\cdot N_+^{(n-k_1)} + N_-^{(k_1)}\cdot N_-^{(n-k_1)}$, and the number of total minus signs is $N_-^{(n)} = N_+^{(k_1)}\cdot N_-^{(n-k_1)} + N_-^{(k_1)}\cdot N_+^{(n-k_1)}$. Due to $N_+^{(k_1)} = N_-^{(k_1)}$ we find $N_+^{(n)} = N_-^{(n)}$. ■

To count all biseparable balanced states we first fix $k$, and also fix the partition in Eq. (5). The number of real equally weighted states where at least one of the two subsystems is balanced is $N_{\rm bisep}(k) = B(2^k,2^{k-1})\cdot 2^{2^{n-k}} + B(2^{n-k},2^{n-k-1})\cdot 2^{2^k} - B(2^k,2^{k-1})\cdot B(2^{n-k},2^{n-k-1})$. This expression is derived by counting the number of balanced functions in the left term times the number of all functions in the right, plus vice versa, minus the terms where both parts are balanced and we have already included it before. Next, we have to sum over all possible bipartitions for fixed $k$ [which leads to the binomial $B(n,k)$ as factor] and then have to sum over all $k$. The only partition where this argument does not hold is the case of $k=n/2$ for even $n$. Here the factor 1/2 is needed to ensure that the partitions are not counted twice. Thus, the number of biseparable balanced states is given by

$$N^{\rm DJ}_{\rm bisep} = \sum_{k=1}^{\lfloor (n-1)/2\rfloor} B(n,k)N_{\rm bisep}(k) + \frac{1}{2}B(n,n/2)N_{\rm bisep}(n/2)\delta_{n/2-\lfloor n/2\rfloor,0}\,. \tag{7}$$

We now want to find $\lim_{n\to\infty} N^{\rm DJ}_{\rm bisep}/N_{\rm bal}$. To this end, it is convenient to write the above expression in the following form:

$$N^{\rm DJ}_{\rm bisep} = \sum_{k=1}^{n-1} B(n,k)[B(2^k,2^{k-1})\cdot 2^{2^{n-k}} - \frac{1}{2}B(2^k,2^{k-1})\cdot B(2^{n-k},2^{n-k-1})]\,. \tag{8}$$

For $n\to\infty$ the largest term in the above equation is the one with $k=1$, and therefore we find that

$$\lim_{n\to\infty} N^{\rm DJ}_{\rm bisep} \leqslant \lim_{n\to\infty} 2(n-1)n\cdot 2^{2^{n-1}}\,. \tag{9}$$

Using this upper bound, we arrive at

$$\lim_{n\to\infty}\frac{N^{\rm DJ}_{\rm bisep}}{N_{\rm bal}} \leqslant \lim_{n\to\infty} 2(n-1)n\cdot 2^{2^{n-1}}/B(2^n,2^{n-1}) = \lim_{n\to\infty}\frac{\sqrt{2\pi}\cdot n^2\cdot 2^{n/2}}{2^{2^{n-1}}}\,. \tag{10}$$

Thus, in the limit of $n\to\infty$ the number of biseparable states among the balanced ones goes to zero, and we conclude that for large $n$ the Deutsch-Jozsa algorithm typically employs genuine multipartite entanglement.

## III. THE GROVER ALGORITHM

In this section we will discuss the case of the Grover algorithm. The state (1) is achieved after the first application of the oracle. In this case the function $f$ has output 1 for entries $x$ that correspond to solutions of the search problem and output 0 for values of $x$ that are not solutions. Let us denote with $M$

the number of solutions, which typically is much smaller than the total number of entries $2^n$. The number of possible states of the form $|\psi_f\rangle$ is $N_M = B(2^n,M)$.

In the case of a single solution $M = 1$ the state (1) corresponds to an equally weighted superposition of all possible computational basis states with the same relative phases, except for a single term, which has relative phase $-1$ with respect to the others. Such a state is fully entangled, because a biseparable state would contain at least two minus signs. Therefore, it is genuine multipartite entangled. The number of possible states with $M = 1$ is clearly $2^n$, because the $-1$ phase can be in front of any of the $2^n$ computational basis states.

In general, we remember that a necessary condition for the state (1) to be fully separable [i.e., of the form (4)] is that the output of $f$ is constant or balanced. Therefore, for nonbalanced or constant functions, namely, whenever $M \neq 0,2^{n-1}$, the state (1) is always entangled. Moreover, in the case of odd $M$ it is never possible to write the state as a tensor product because this would lead to an even number of $-1$ relative phases in the state $|\psi_f\rangle$. Therefore, whenever the number of solutions $M$ is odd, the state $|\psi_f\rangle$ is fully entangled.

Let us now consider the case $M = 2$. Here the state (1) can be either biseparable or entangled. Actually, the only possibility of writing it as tensor product would be in the form

$$|\psi_{\text{bisep}}\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \otimes |\psi_{\text{ent},n-1}\rangle \ , \tag{11}$$

where $|\psi_{\text{ent},n-1}\rangle$ represents a fully entangled state of $n-1$ qubits, of the form (1) and with just one relative phase $-1$ in the superposition, and the partition is arbitrary. If the state cannot be written in this form in any partition, then it is fully entangled. As mentioned above, the total number of possible states with $M = 2$ is $B(2^n,2)$, while the number of biseparable states among these is $n2^{n-1}$. Therefore, the fraction of biseparable states for $M = 2$ is exponentially small in the asymptotic limit. In other words, for large $n$ and $M = 2$ the Grover algorithm typically employs genuine multipartite entanglement.

Let us now consider the case $M = 4$. The state $|\psi_f\rangle$ in this case is biseparable, triseparable, or fully entangled. Actually, it could be factorized in the triseparable form,

$$|\psi_{3-\text{sep}}\rangle \equiv \tfrac{1}{2}(|0\rangle + |1\rangle)^{\otimes 2} \otimes |\psi_{\text{ent},n-2}\rangle \ , \tag{12}$$

where $|\psi_{\text{ent},n-2}\rangle$ represents a fully entangled state of $n-2$ qubits, of the form (1) and with just one relative phase $-1$ in the superposition, and the partition is again arbitrary. The number of possible triseparable states of the above form is $2^{n-2}B(n,2)$. The only other possibility of factoring it is in the biseparable form (11), where $|\psi_{\text{ent},n-1}\rangle$ represents a fully entangled state of $n-1$ qubits, of the form (1) and with two components with $-1$ relative phases in the superposition. If the state cannot be written in the above biseparable form or in the triseparable form (12) for any partition, then it is fully entangled.

The total number of biseparable states for $M = 4$ [written as tensor product either in the triseparable form (12) or in the form (11)] is $N^G_{\text{bisep}} = nB(2^{n-1},2)$. The fraction of biseparable states is then given by

$$\lim_{n\to\infty} \frac{N^G_{\text{bisep}}}{N_{M=4}} = \lim_{n\to\infty} \frac{nB(2^{n-1},2)}{B(2^n,4)} \simeq 0 \ , \tag{13}$$

namely, the states employed are typically genuine multipartite entangled.

The above argument can be generalized to values of $M$ that are powers of 2: for $M = 2^k$, the initial state $|\psi_f\rangle$ can be biseparable, triseparable, $\dots,(k+1)$-separable, or fully entangled. When the state is $k+1$-separable it has to be of the form

$$|\psi_{k+1-\text{sep}}\rangle \equiv \frac{1}{2^{k/2}}(|0\rangle + |1\rangle)^{\otimes k} \otimes |\psi_{\text{ent},n-k}\rangle \ , \tag{14}$$

where $|\psi_{\text{ent},n-k}\rangle$ is a fully entangled state of $n-k$ qubits with a single term in the superposition having relative phase $-1$. The reason for this structure is as follows: assume that the $k$ parties would contain entanglement; then the number $M$ of solutions, according to the lemma, would be at least $M \geqslant 2^{n/2}$, while we require $M \ll 2^n$. The number of states of the form (14) is $2^{n-k}B(n,k)$.

When the state is $k$-separable it has to be of the form

$$|\psi_{k-\text{sep}}\rangle \equiv \frac{1}{2^{(k-1)/2}}(|0\rangle + |1\rangle)^{\otimes k-1} \otimes |\psi_{\text{ent},n-k+1}\rangle \ , \tag{15}$$

where now $|\psi_{\text{ent},n-k+1}\rangle$ is a fully entangled state of $n-k+1$ qubits with two components having $-1$ relative phase. In general, for $M = 2^k$, the state $|\psi_f\rangle$ can be $j$-separable, with $j \leqslant k+1$, or fully entangled.

For a generic even $M = 2^q(2p+1)$, the state $|\psi_f\rangle$ can be always biseparable or fully entangled. In particular, the state can then be $j$-separable, with all values of $j$ ranging from 2 to $q+1$, or fully entangled. The number of biseparable states for even $M$ is in general given by $N^G_{\text{bisep}}(M) = nB(2^{n-1},M/2)$. Therefore, the fraction of biseparable states is given by

$$\lim_{n\to\infty} \frac{N^G_{\text{bisep}}(M)}{N_M} = \lim_{n\to\infty} \frac{nB(2^{n-1},M/2)}{B(2^n,M)} \simeq 0 \ , \tag{16}$$

where we consider $q$ and $p$ finite and fixed. We can then conclude that for any $M \ll N$ (as mentioned above, in our analysis it is sufficient that $M < 2^{n/2}$) the states are typically multipartite entangled.

## IV. THE SIMON ALGORITHM

In this section we will consider the Simon algorithm [8]. In this case the function to be evaluated is promised to be a $\{0,1\}^n \to \{0,1\}^n$ periodic $2 \to 1$ function, and the task is to evaluate the period $r$ ($r$ is an $n$-bit string, with $r \neq 0$) with the smallest number of evaluations. In other words, in Simon's case $f(x) = f(y)$ if and only if $x = y \oplus r$. The first register, as in the previous cases, is composed of $n$ qubits prepared in state $|\psi_0\rangle$, while the target register is now composed of another set of $n$ qubits, which are all prepared in state $|0\rangle$.

After the function evaluation step (3), the global state of the two registers takes the form

$$\left|\psi^{(2)}_{\text{Simon}}\right\rangle \equiv \frac{1}{\sqrt{2^{n-1}}} \sum_{i=1}^{2^{n-1}} (|x_i\rangle + |x_i + r\rangle)|f(x_i)\rangle \ , \tag{17}$$

where $x_i$ is the set of $2^{n-1}$ input values leading to different outputs. Notice that the above state is always entangled between the two registers. The next step is a measurement on the second register, after which the state of the first register takes the simple form

$$|\psi_{\text{Simon}}\rangle \equiv \frac{1}{\sqrt{2}}(|\bar{x}\rangle + |\bar{x}+r\rangle)\,, \tag{18}$$

where $\bar{x}$ is now a random value among the $x_i$'s. We will now study the entanglement properties of the states of the form (18). Notice that, by keeping $r$ fixed and changing $\bar{x}$ in the above form, the entanglement properties of the state do not change because by applying just local operations (of the type $\sigma_x$) we can reach all the states of the above form (with different $\bar{x}$ and same $r$). We can then for simplicity analyze the properties of these states by choosing the particular value $\bar{x} = 0$, namely,

$$|\psi_{\text{Simon},0}\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + |r\rangle)\,. \tag{19}$$

Notice that the number of possible different states of the above form, corresponding to all the possible nonvanishing values of $r$, is $2^n - 1$. If $r$ contains a single value 1, i.e., $wt(r) = 1$ [$wt(r)$ is the weight of the binary string $r$, namely, the number of 1's that it contains] then the state $|\psi_{\text{Simon},0}\rangle$ is fully separable ($\in S_n$), because it is of the form $1/\sqrt{2}(|0\rangle + |1\rangle)|0\rangle \cdots |0\rangle$. There are $n$ possible states of this type, corresponding to the different strings of length $n$ with weight 1.

If $wt(r) = 2$, then the state (19) contains two-qubit entanglement ($\in S_{n-1}$). The number of states of this form is $B(n,2)$. This simple counting argument can be generalized to the case of an arbitrary weight for $r$: if $wt(r) = k$ the state (19) belongs to $S_{n-k+1}$ and there are $B(n,k)$ of them. The case of maximum weight is $wt(k) = n$ and then the state is $n$-partite entangled, of the GHZ form. Notice that the most populated class of states corresponds to values of the period $r$ with $wt(r) = \lfloor n/2 \rfloor$, i.e., typically half of the qubits are entangled with each other.

## V. CONCLUSIONS

In this paper we have elucidated the role of multipartite entanglement in the quantum algorithms of Deutsch-Jozsa, Grover, and Simon by studying the properties of the family of "real equally weighted states." For the Deutsch-Jozsa algorithm, multipartite entanglement within the first register is needed to accommodate all possible (balanced) functions. We have shown that the fraction of balanced functions corresponding to biseparable states decreases exponentially with the number of qubits. In this sense most balanced functions involve genuine multipartite entanglement. In the Grover algorithm, we have shown that the entanglement properties of the initial state of the first register depend on the number of solutions, and we have demonstrated that such a state is also typically multipartite entangled, when a small number of items is searched for. In the Simon algorithm the situation is slightly different: in general the first register and the target register are entangled. Moreover, the kind of entanglement within the first register after the measurement of the target register depends on the weight of the period $r$: for increasing weight it involves an increasing number of qubits. For large $n$, the states employed typically involve entanglement among half of the constituent qubits. We have thus shown that multipartite entanglement is an important property in the considered quantum algorithms.

We point out that in this analysis we have not performed any quantitative estimate of the multipartite entanglement occurring in the considered algorithms, or of their simulatability features [9]. These are interesting open questions, which will be the object of future investigations.

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