Analysis of Grover’s quantum search algorithm as a dynamical system

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Abstract

Grover’s quantum search algorithm is analyzed for the case in which the initial state is an arbitrary pure quantum state $|\phi\rangle$ of $n$ qubits. It is shown that the optimal time to perform the measurement is independent of $|\phi\rangle$, namely, it is identical to the optimal time in the original algorithm in which $|\phi\rangle = |0\rangle$, with the same number of marked states, $r$. The probability of success $P_s$ is obtained, in terms of the amplitudes of the state $|\phi\rangle$, and is shown to be independent of $r$. A class of states, which includes fixed points and cycles of the Grover iteration operator is identified. The relevance of these results in the context of using the success probability as an entanglement measure is discussed. In particular, the Groverian entanglement measure, previously limited to a single marked state, is generalized to the case of several marked states.
I. INTRODUCTION

Grover’s quantum search algorithm \[1, 2\] exemplifies the potential speed-up offered by quantum computers. It also provides a laboratory for the analysis of quantum algorithms and their implementation. The problem addressed by Grover’s algorithm can be viewed as trying to find a marked element in an unsorted database of size $N$. While a classical computer would need, on average, $N/2$ database queries (and $N$ queries in the worst case) to solve this problem, a quantum computer using Grover’s algorithm, would accomplish the same task using merely $O(\sqrt{N})$ queries. The importance of Grover’s result stems from the fact that it proves the enhanced power of quantum computers compared to classical ones for a whole class of oracle-based problems, for which the bound on the efficiency of classical algorithms is known. Moreover, it was shown \[3\] that Grover’s algorithm is as efficient as theoretically possible \[4\]. A variety of applications were developed, in which the algorithm is used in the solution of other problems \[5, 6, 7, 8, 9, 10, 11\]. Experimental implementations of Grover’s algorithm were constructed using nuclear magnetic resonance (NMR) \[12, 13\] as well as an optical device \[11\].

Several generalizations of Grover’s original algorithm have been developed. The case in which there are several marked states was studied in Ref. \[15\]. It was shown that when there are $r$ marked states, Grover’s algorithm would be able to find one of them after $T = O(\sqrt{N/r})$ queries. A further generalization was obtained by allowing the replacement of the Hadamard transform, used in the original setting, by an arbitrary (but constant) unitary transformation \[16, 17, 18\], as well as by the replacement of the $\pi$ inversion by an arbitrary (but constant) phase rotation \[19\].

Another generalization was obtained by allowing the replacement of the uniform superposition of all basis states, used as the initial state of the algorithm in the original setting, by an arbitrary pure \[20, 21\] or mixed \[22\] quantum state. In this case the probability of success of the algorithm, $P_s$, may be reduced, depending on the initial state. Recently it was shown that this generalization gives rise to an entanglement monotone that can be used to quantify the entanglement in pure states of multiple qubits \[23\].

In this paper we provide a comprehensive analysis of the dynamical behavior and the success probability of the quantum search algorithm for arbitrary initial pure quantum states. We show that for a given initial state, $|\phi\rangle$, the success probability does not depend
on the number of marked states used in the algorithm. We provide an explicit expression for \( P_s \) in terms of the amplitudes of the initial state, and discuss a simple geometrical interpretation of it. We then use this approach to calculate \( P_s \) for states that exhibit various symmetries, as well as states that typically appear in quantum algorithms. Two special classes of states are identified: fixed points, namely states that remain invariant under the Grover iteration as well as two-cycles. The implications of the results in the context of entanglement measures for quantum states of multiple qubits are discussed.

The paper is organized as follows. In Sec. II we briefly describe the algorithm. The algorithm in the case of an arbitrary initial quantum state is studied in Sec. III, where an expression for \( P_s \) is obtained and shown to be independent of \( r \), and fixed points and cycles are identified. The results are discussed in Sec. IV and summarized in Sec. V.

II. THE QUANTUM SEARCH ALGORITHM

Consider a search space \( D \) containing \( N \) elements. We assume, for convenience, that \( N = 2^n \), where \( n \) is an integer. In this way, we may represent the elements of \( D \) using an \( n \)-qubit register containing the indices, \( i = 0, \ldots, N - 1 \). We assume that a subset of \( r \) elements in the search space are marked, that is, they are solutions of the search problem. The distinction between the marked and unmarked elements can be expressed by a suitable function, \( f : D \rightarrow \{0, 1\} \), such that \( f = 1 \) for the marked elements, and \( f = 0 \) for the rest. The search for a marked element now becomes a search for an element for which \( f = 1 \). To solve this problem on a classical computer one needs to evaluate \( f \) for each element, one by one, until a marked state is found. Thus, on average, \( N/2 \) evaluations of \( f \) are required and \( N \) in the worst case. For a quantum computer, on which \( f \) to be evaluated coherently, it was shown that a sequence of unitary operations called Grover’s algorithm can locate a marked element using only \( O(\sqrt{N/r}) \) coherent queries of \( f \).

To describe the operation of the quantum search algorithm we first introduce a register, \( |i\rangle = |i_1 \ldots i_n\rangle \), of \( n \) qubits, and an ancilla qubit, \( |q\rangle \), to be used in the computation. We also introduce a quantum oracle, a unitary operator \( O \) which functions as a black box with the ability to recognize solutions to the search problem. The oracle performs the following
unitary operation on computational basis states of the register, \( |i\rangle \), and the ancilla, \( |q\rangle \):

\[
O |i\rangle |q\rangle = |i\rangle |q \oplus f(i)\rangle
\]

(1)

where \( \oplus \) denotes addition modulo 2. The oracle recognizes marked states in the sense that if \( |i\rangle \) is a marked element of the search space, namely \( f(i) = 1 \), the oracle flips the ancilla qubit from \( |0\rangle \) to \( |1\rangle \) and vice versa, while for unmarked states the ancilla is unchanged. The ancilla qubit is initially set to the state

\[
|\rangle_q = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle).
\]

(2)

With this choice, the action of the oracle is:

\[
O|i\rangle |\rangle_q = (-1)^{f(i)} |i\rangle |\rangle_q.
\]

(3)

Thus, the only effect of the oracle is to apply a phase of \(-1\) if \(x\) is a marked basis state, and no phase change if \(x\) is unmarked. Since the state of the ancilla does not change, one may omit it and write the action of the oracle as \(O|x\rangle = (-1)^{f(x)} |x\rangle\).

Grover’s search algorithm may be described as follows: Given a black box oracle \(O\), whose action is defined by Eq. (1) and a register of \(n+1\) qubits in the state \(|0\rangle \otimes |0\rangle_q\), the following procedure is performed:

1. **Initialization:** Apply a Hadamard gate \(H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \) to each qubit in the register, and the gate \(HX\) to the ancilla, where \(X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\) is the NOT gate, and we write matrices with respect to the computational basis \((|0\rangle, |1\rangle)\). The resulting state is:

\[
|\eta\rangle |\rangle_q.
\]

(4)

where

\[
|\eta\rangle = \frac{1}{\sqrt{N}} \sum_{i=0}^{N-1} |i\rangle.
\]

(5)

2. **Grover Iterations:** Repeat the following operation \(\tau\) times (where \(\tau\) is an integer given below).
(a) Apply the oracle, which has the effect of rotating the marked states by a phase of \( \pi \) radians. Since the ancilla is always in the state \( |\rangle_q \) the effect of this operation may be described by the following unitary operator

\[
I_f^\pi = \sum_{i=0}^{N-1} (-1)^{f(i)} |i\rangle\langle i|,
\]

acting only on the register.

(b) (i) apply the Hadamard gate on each qubit in the register; (ii) Rotate the \( |00\ldots0\rangle \) state of the register by a phase of \( \pi \) radians. This rotation is similar to 2(a), except for the fact that here it is performed on a known state. It takes the form

\[
I_0^\pi = -2|0\rangle\langle 0| + \sum_{i=0}^{N-1} |i\rangle\langle i|,
\]

where the second term on the right hand side is the identity operator, denoted by \( I \); (iii) Apply the Hadamard gate again on each qubit in the register.

The resulting operation is

\[
-H^\otimes n I_0^\pi H^\otimes n = -I + 2H^\otimes n |0\rangle\langle 0| H^\otimes n = -I + |\eta\rangle\langle \eta|.
\]

When this operator is applied on the state \( \sum_i a_i |i\rangle \) it results in the state \( \sum_i (2\bar{a} - a_i) |i\rangle \), where \( \bar{a} = \sum_i a_i/N \). Thus, each amplitude is rotated by \( \pi \) around the average of all amplitudes of the quantum state.

The combined operation on the register in one Grover iteration is described by

\[
U_G = -H^\otimes n I_0^\pi H^\otimes n I_f^\pi.
\]

3. Measure the register in the computational basis.

The optimal number of iterations is

\[
\tau = \left\lfloor \frac{\pi}{4} \sqrt{\frac{N}{r}} \right\rfloor,
\]
where \(|x|\) is the largest integer which is smaller than \(x\). Moreover, at this optimal time a marked state can be found with almost certainty, or more precisely with probability

\[
P_s = 1 - O\left(\frac{1}{\sqrt{N}}\right).
\]

(11)

With this performance, Grover’s algorithm was found to be optimal in the sense that it is as efficient as theoretically possible \([4]\).

Note that the probability \(P \approx 1\) can be achieved only for specific initial states such as the one produced in step 1 of the algorithm above. If this starting state is replaced by an arbitrary quantum state, the probability of success, \(P_s\), is reduced \([20, 21]\). In the next Section we analyze the operation of the algorithm in the case that the initial state is an arbitrary pure quantum state \(|\phi\rangle\). The time evolution of the quantum state during the Grover iterations is examined, for a specific choice of the marked states. Special states that exhibit fixed points and cycles under Grover iterations are identified. A closed form expression for \(P_s\) is obtained, and a geometrical interpretation for it is presented. It is shown that for a given state \(|\phi\rangle\), the success probability does not depend on the number of marked states. Finally, some specific quantum states are examined and their utility as initial states for Grover’s algorithm is obtained.

III. GROVER’S ALGORITHM WITH AN ARBITRARY PURE INITIAL STATE

A. The initial state

Consider an arbitrary pure quantum state \(|\phi\rangle\) of \(n\) qubits, to be used as the initial state in Grover’s algorithm. It can be expressed by

\[
|\phi\rangle = \sum_{i=0}^{N-1} a_i(0)|i\rangle,
\]

(12)

where the amplitudes \(a_i(0), \ i = 0, \ldots, N - 1\) are complex numbers that satisfy

\[
\sum_{i=0}^{N-1} |a_i(0)|^2 = 1,
\]

(13)

and \(N = 2^n\). The distribution of these amplitudes can be characterized by its moments.
The first moment (or average) of the amplitudes is
\[
\overline{a(0)} = \frac{1}{N} \sum_{i=0}^{N-1} a_i(0). \tag{14}
\]
The second moment
\[
\overline{|a(0)|^2} = \frac{1}{N} \sum_{i=0}^{N-1} |a_i(0)|^2 \tag{15}
\]
satisfies \(|a(0)|^2 = 1/N\), for any state |φ⟩, due to the normalization condition \[(13)\). The standard deviation of the amplitude distribution is given by
\[
\sigma_a^2(0) = \frac{1}{N} \sum_{i=0}^{N-1} |a_i(0) - \overline{a(0)}|^2. \tag{16}
\]
Using the equality
\[
\sigma_a^2(0) = |a(0)|^2 - |\overline{a(0)}|^2 \tag{17}
\]
we obtain that
\[
\sigma_a^2(0) = \frac{1}{N} - |\overline{a(0)}|^2. \tag{18}
\]
This result can be used to identify two limits. One limit is the equal superposition state, in which \(a_i(0) = 1/\sqrt{N}\) for \(i = 0, \ldots, N - 1\). In this state \(\overline{a(0)} = 1/\sqrt{N}\) and \(\sigma_a(0) = 0\). In the opposite limit there is a large family of states for which \(a(0) = 0\). In this case \(\sigma_a(0) = 1/\sqrt{N}\), which is the largest value that \(\sigma_a(0)\) can take.

B. Recursion equations for a pre-defined set of marked states

Consider Grover’s algorithm, searching for one of \(r\) marked states where the initial state is |φ⟩. Denote the set of indices of the marked states by \(M\). The amplitudes of the marked states will thus be \(a_i, \ i \in M\). In some cases below, we will denote the marked states by \(|m_1⟩, \ldots, |m_r⟩\) and their amplitudes by \(a_{m_1}(0), \ldots, a_{m_r}(0)\). The complementary set, which includes the indices of the unmarked states, will be denoted by \(\overline{M}\).

The time evolution of the amplitudes of the marked and unmarked states during the Grover’s iterations with an arbitrary pure quantum state as the initial state, was studied in
Ref. [21]. Starting from the state $|\phi\rangle$, the amplitudes obtained after $t$ Grover iterations are denoted by $a_i(t)$, $i = 0, \ldots, N - 1$.

For a given choice of the marked states, one can consider separately the averages and standard deviations of the sets of marked and unmarked states at time $t$. The averages will be

$$a_m(t) = \frac{1}{r} \sum_{i \in M} a_i(t)$$

for the marked states, and

$$a_u(t) = \frac{1}{N - r} \sum_{i \in M} a_i(t)$$

for the unmarked states. The standard deviations will be

$$\sigma_m^2(t) = \frac{1}{r} \sum_{i \in M} |a_i(t) - a_m(t)|^2$$

for the marked states, and

$$\sigma_u^2(t) = \frac{1}{N - r} \sum_{i \in M} |a_i(t) - a_u(t)|^2.$$  

for the unmarked states.

Each Grover iteration consists of two steps. In the first step the phases of all the marked amplitudes are rotated by $\pi$, namely $a_i \to -a_i$, $i \in M$. In the second step all the amplitudes are rotated by $\pi$ around their average, namely $a_i \to 2\bar{a} - a_i$, $i = 0, \ldots, N - 1$. Using these properties, the time dependence was found to be described by the recursion equations [21]

$$a_i(t + 1) = C(t) + a_i(t) \quad i \in M$$

$$a_i(t + 1) = C(t) - a_i(t) \quad i \in \overline{M}$$

and

$$C(t) = \frac{2}{N} \left[ (N - r)\overline{a_u(t)} - r\overline{a_m(t)} \right].$$
It was also shown that the standard deviations of the amplitude distributions of the marked and unmarked states are constants of motion, namely $\sigma_m(t) = \sigma_m(0)$ and $\sigma_u(t) = \sigma_u(0)$ at any time $t$.

C. Solution of the recursion equations

Consider a quantum search with $r$ marked states, using an arbitrary quantum state $|\phi\rangle$ as the initial state. It was shown in Ref. [21] that the time evolution of the amplitudes is given by

$$a_i(t) = a_m(t) + \Delta a_i : i \in M$$

$$a_i(t) = a_u(t) + (-1)^t \Delta a_i : i \in \overline{M},$$

where

$$a_m(t) = \sqrt{N-r} \alpha \sin(\omega t + \delta)$$

$$a_u(t) = \alpha \cos(\omega t + \delta)$$

and

$$\Delta a_i = a_i(0) - a_m(0) : i \in M$$

$$\Delta a_i = a_i(0) - a_u(0) : i \in \overline{M}.$$  

The parameters $\alpha$ and $\delta$ are given by

$$\alpha = \sqrt{\frac{\alpha_u(0)^2 + \frac{r}{N-r} \alpha_m(0)^2}{\sqrt{N-r} \alpha_u(0) + i \sqrt{r} \alpha_m(0)}}$$

$$\exp(2i\delta) = \frac{\sqrt{N-r} \alpha_u(0) + i \sqrt{r} \alpha_m(0)}{\sqrt{N-r} \alpha_u(0) - i \sqrt{r} \alpha_m(0)},$$

where $-\pi/2 \leq \text{Re}(\delta) < \pi/2$. Furthermore, it was found that if a measurement is taken after $t$ iterations, the probability to find one of the marked states is given by

$$P(t) = P_0 - \Delta P \cos^2[\omega t + \text{Re}(\delta)]$$
where

\[ P_0 = 1 - (N - r)\sigma_u^2 - \frac{1}{2}K \]  

(30)
is the highest probability of success that can be achieved for the specific choice of the set of marked states denoted by M (if the measurement is taken at the optimal time). The parameter \( K \) takes the form

\[ K = (N - r)\left|a_u(0)\right|^2 + r\left|a_m(0)\right|^2 - \left|(N - r)a_u(0)^2 + ra_m(0)^2\right|. \]  

(31)
The coefficient of the time dependent term is

\[ \Delta P = \left|(N - r)a_u(0)^2 + ra_m(0)^2\right|. \]  

(32)
The frequency \( \omega \) given by

\[ \cos \omega = 1 - \frac{2r}{N}, \]  

(33)
or approximately by \( \omega = 2\sqrt{r/N} \) where \( r \ll N \). The function \( P(t) \) is a sinusoidal function. In the analysis of the efficiency of the algorithm we are interested in the largest value \( P_0 \) that this function may reach during its cycle. We are also interested in the number of iterations that it would take to reach this maximum for the first time, from the given initial state. This optimal number of iterations, for the given set, M of marked states is given by

\[ \tau_M = \left\lfloor \frac{1}{2}\sqrt{\frac{N}{r}\left(\frac{\pi}{2} - \text{Re}(\delta)\right)} \right\rfloor. \]  

(34)
Note that for \( 0 \leq \text{Re}(\delta) < \pi/2 \), \( \tau_M \leq \tau \) namely the optimal number of iterations is equal or smaller than for the initial state \( |\eta\rangle \). On the other hand, for \( -\pi/2 \leq \text{Re}(\delta) < 0 \) the optimal number of iterations \( \tau_M \) is larger than \( \tau \). Note that within this analysis, in which the set of marked states is assumed to be known, it would be more efficient for \( -\pi/2 \leq \text{Re}(\delta) < 0 \), to apply the Grover iterations \([9]\) in reverse order. Of course this does not apply to the actual search in which the marked states are unknown.

There are several issues to consider about the probability \( P_0 \). First, the case that we considered so far is not the real search. This is due to the fact that in the derivation of Eq. (29) it was assumed that the identities of the marked states and their amplitudes are
known. In order to obtain the probability of success of an actual search one needs to average Eq. (29) over all possible sets of the $r$ marked states. In the case of one marked state this yields an average over $N$ possibilities. In general, for $r$ marked states the number of possible sets is given by the binomial coefficient \( \binom{N}{r} \). Averaging over all these possibilities yields \( \langle a_m(0) \rangle \), which is the average of $a_m(0)$ over all possible sets of $r$ marked states. This average is used as a small parameter in the series expansion that provides the average of $P(t)$ over all these possible choices of the marked states.

Consider the constant $K$ in Eq. (31). For an initial state $|\phi\rangle$ in which all the amplitudes are real, there is an exact cancellation and $K = 0$. Clearly, this simplifies the calculation of $P_0$ significantly. In case that the amplitudes are complex, and the phases of $a_m(0)$ and $a_u(0)$ are different, $K$ may be nonzero. It is easy to see that it is bounded by $0 \leq K \leq \min\{2r \left| a_m(0) \right|^2, 2(N-r) \left| a_u(0) \right|^2 \}$. Consider, for example, the case of a single marked state. For a specific choice of $m_1$, the constant $K$ can take any value in the range $0 \leq K \leq 1$. However, averaging it over all the $N$ possible choices of the marked state, it is easy to see that $K$ is reduced to order $1/N$.

For a given choice of the set of marked states, the optimal time to measure is found to depend on the initial state according to Eq. (34). However, by averaging $P(t)$ [Eq. (29)] over all possible choices of the set of marked states, Eq. (30) is replaced by

\[
P_0 = 1 - N\sigma_a^2 + O \left( \frac{1}{\sqrt{N}} \right),
\]

and using Eq. (18) we obtain

\[
P(t) = N \left| a(0) \right|^2 \sin^2(\omega t) + O \left( \frac{1}{\sqrt{N}} \right).
\]

Therefore, for any initial state $|\phi\rangle$, the optimal number of iterations to be performed before taking the measurement remains the same, namely $\tau$ [Eq. (10)]. The probability of success is $P_s = N \left| a(0) \right|^2$. The averaging process that leads to this result is rather tedious. In the next Sections we will present a more elegant approach for the calculation of $P_s$.

### D. Fixed points and cycles

Typically, the function $P(t)$ is a quasi-periodic function since, generically, the frequency $\omega/(2\pi)$ is incommensurate with the sequence of integers counting the Grover iterations. A
periodic (rather than quasi-periodic) cycle of the amplitudes is obtained when the frequency \( \omega \) is a rational product of \( 2\pi \). This condition is satisfied when

\[
\cos^{-1}\left(1 - 2\frac{r}{N}\right) = \frac{p}{q}\pi.
\]

One example of such periodic cycle appears when \( N/r = 4 \). In this case \( \omega = \pi/3 \), and the cycle is of period 6.

For some initial states and specific choices of the set of marked states, Grover’s algorithm does not provide any enhancement of the probability to obtain a marked state. Such situations appear when \( \Delta P = 0 \), thus the success probability \( P(t) \) becomes a constant. The condition for \( \Delta P = 0 \) can be expressed by

\[
\sqrt{\frac{N - r}{r}} a_m(0) = \pm i \sqrt{N - r} a_u(0).
\]

Under this condition the amplitude \( \alpha = 0 \), and thus \( a_m(t) = 0 \) and \( a_u(t) = 0 \). It is easy to see from the geometrical description of the algorithm that in this case the operator \( U_G \) exhibits cycles of period 2, namely

\[
U_G^2 |\phi\rangle = |\phi\rangle.
\]

The condition for a two-cycle is simply \( a_m(0) = 0 \) and \( a_u(0) = 0 \). This is due to the fact that under this condition the amplitudes of the marked states are invariant under \( U_G \), while those of the unmarked states change sign at each iteration (what matters is the relative phase of \( \pi \) between the marked and unmarked states, while the global phase can be ignored).

We will also consider fixed points of \( U_G \), namely states that satisfy

\[
U_G |\phi\rangle = |\phi\rangle.
\]

The set of fixed points of \( U_G \) consists of two classes: (a) states for which \( a_m(0) = 0 \) and \( a_i(0) = 0 \) for each of the unmarked states; (b) states for which \( a_m(i) = 0 \) for each of the marked states and \( a_u(0) = 0 \). In the case of a single marked state, \( |m_1\rangle \), a fixed point is obtained when \( a_m(i) = 0 \) and \( a_u(0) = 0 \) (where at least two of the unmarked amplitudes are non-zero).
Consider the case of two marked states, $|m_1\rangle$ and $|m_2\rangle$. The state

$$|\phi\rangle = \frac{1}{\sqrt{2}} (|m_1\rangle - |m_2\rangle)$$

is a fixed point of $U_G$ because the amplitudes of all the unmarked states vanish and the average amplitude of the marked states vanishes as well. In the case of $r$ marked states, $|m_1\rangle, \ldots, |m_r\rangle$, the states

$$|\phi\rangle = \sum_{i=1}^{r} a_{m_i}(0)|m_i\rangle,$$

where $a_{m}(0) = 0$, are fixed points of $U_G$.

We conclude that with the exception of those periodic cycles with periods related to the frequency $\omega$, the only possible cycles of $U_G$ are the fixed points and cycles of period 2, discussed above.

### E. The probability of success for one marked state

The initialization step of the original algorithm leads to the state $|\eta\rangle$, given by Eq. (5). Consider the case that there are $r$ marked states, $|m_i\rangle$, $i = 1, \ldots, r$. The operation of the algorithm, using the optimal initial state, $|\eta\rangle$, and performing the optimal number of iterations, $\tau$, can be expressed by

$$U_G^\tau |\eta\rangle = \frac{1}{\sqrt{r}} \sum_{i=1}^{r} |m_i\rangle + O \left( \frac{1}{\sqrt{N}} \right).$$

We will now examine the case in which the initial state is an arbitrary pure quantum state $|\phi\rangle$ of $n$ qubits. The purpose of the algorithm is to find one of the marked states, which are not known in advance. As we have seen in the previous Section, the optimal number of iterations is $\tau$, which is independent of the initial state $|\phi\rangle$. The final state, just before the measurement of the register, will thus be $U_G^\tau |\phi\rangle$. We will now calculate the probability that a measurement of this state will yield one of the marked states. For simplicity, we will first consider the case of one marked state $|m_1\rangle$. In this case, for the initial state $|\eta\rangle$ we obtain

$$U_G^\tau |\eta\rangle = |m_1\rangle + O \left( \frac{1}{\sqrt{N}} \right).$$
For an arbitrary initial state $|\phi\rangle$, the resulting state will be $U_G^\tau |\phi\rangle$, and the probability that a measurement of this state will yield the marked state $|m_1\rangle$ is

$$P_s = |\langle m_1 | U_G^\tau |\phi\rangle|^2 + O \left( \frac{1}{\sqrt{N}} \right).$$  \hspace{1cm} (45)$$

Note that Eq. (44) can be written in the form

$$\langle m_1 | U_G^\tau = \langle \eta | + O \left( \frac{1}{\sqrt{N}} \right).$$  \hspace{1cm} (46)$$

Inserting this equation into (45) we obtain that

$$P_s = |\langle \eta | \phi\rangle|^2 + O \left( \frac{1}{\sqrt{N}} \right),$$  \hspace{1cm} (47)$$

namely, $P_s$ is given by the overlap of $\phi$ with the equal superposition $|\eta\rangle$.

Note that in the analysis above we used an arbitrary marked state $|m_1\rangle$. Since the marked state is not known, the calculation of $P_s$ should be done by averaging Eq. (45) over all the $N$ possible choices of the marked state. It will thus take the form

$$P_s = \frac{1}{N} \sum_{i=0}^{N-1} |\langle i | U_G^\tau |\phi\rangle|^2 + O \left( \frac{1}{\sqrt{N}} \right),$$  \hspace{1cm} (48)$$

where in each of the $N$ terms the operator $U_G$ is constructed such that the marked state is the corresponding state $|i\rangle$. It turns out that this averaging is not really necessary, because all the $N$ terms in this sum are identical [up to corrections of order $O(1/\sqrt{N})$].

Eq. (47) can be used in order to express the success probability $P_s$ in terms of the amplitudes of $|\phi\rangle$. To this end we will express the states $|\eta\rangle$ and $|\phi\rangle$ in terms of their amplitudes, according to Eqs. (5), and (12), respectively, and obtain

$$P_s = N \left| \bar{a}(0) \right|^2 + O \left( \frac{1}{\sqrt{N}} \right).$$  \hspace{1cm} (49)$$

Clearly, $P_s$ turns out to depend only on the first moment of the distribution of the amplitudes. Initial states that exhibit high values of $P_s$ are those for which the average amplitude $\bar{a}$ is large (in absolute value).
F. The probability of success for two marked states

Consider the quantum search algorithm with an initial state $|\phi\rangle$ and two marked states, $|m_1\rangle$ and $|m_2\rangle$. The probability that the algorithm will yield one of the marked states is

$$P_s = |\langle m_1 | U^r_G | \phi \rangle|^2 + |\langle m_2 | U^r_G | \phi \rangle|^2 + O\left(\frac{1}{\sqrt{N}}\right).$$

(50)

In this case, the operation of the algorithm on the initial state $|\eta\rangle$ can be described by

$$U^r_G |\eta\rangle = \frac{1}{\sqrt{2}}(|m_1\rangle + |m_2\rangle) + O\left(\frac{1}{\sqrt{N}}\right).$$

(51)

or

$$\frac{1}{\sqrt{2}}(|m_1\rangle + |m_2\rangle)U^r_G = |\eta\rangle + O\left(\frac{1}{\sqrt{N}}\right).$$

(52)

Unlike the case of a single marked state, this equation cannot be applied directly for the evaluation of $P_s$. The reason is that $P_s$ is determined by the overlaps of $U^r_G |\phi\rangle$ with each one of the marked states separately and not with their superposition. To overcome this difficulty, we will use the following identity:

$$|\langle m_1 | \psi \rangle|^2 + |\langle m_1 | \psi \rangle|^2 = \frac{1}{2} |(\langle m_1 | + \langle m_2 |)\psi\rangle|^2 + \frac{1}{2} |(\langle m_1 | - \langle m_2 |)\psi\rangle|^2,$$

(53)

where $|\psi\rangle$ is an arbitrary quantum state of $n$ qubits. Using this identity, we can write

$$|\langle m_1 | U^r_G | \phi \rangle|^2 + |\langle m_2 | U^r_G | \phi \rangle|^2 = \frac{1}{2} |(\langle m_1 | + \langle m_2 |)U^r_G | \phi \rangle|^2 + \frac{1}{2} |(\langle m_1 | - \langle m_2 |)U^r_G | \phi \rangle|^2.$$  

(54)

In both terms on the right-hand size, we now apply the operator $U^o_G$ to the left. In the first term, according to Eq. (52), this gives rise to the state $|\eta\rangle$. In the second term, the state on the left-hand size of $U^r_G$ is a fixed point of this operator and thus remains unchanged. Therefore

$$|\langle m_1 | U^r_G | \phi \rangle|^2 + |\langle m_2 | U^r_G | \phi \rangle|^2 = |\langle \eta | \phi \rangle|^2 + \frac{1}{2} |(\langle m_1 | - \langle m_2 |)\phi\rangle|^2.$$  

(55)

Note that the first term on the right-hand size does not depend on the choice of the two marked states, similarly to what we obtained for a single marked state. Therefore, the averaging over all the possible choices of two marked states out of $N$ basis states is not
necessary. However, the second term does depend on the choice of \( |m_1 \rangle \) and \( |m_2 \rangle \). Thus the averaging is required, resulting in

\[
P_s = |\langle \eta | \phi \rangle|^2 + \frac{1}{N(N-1)} \sum_{m_1,m_2=0}^{N-1} |\langle m_1 | - \langle m_2 | \phi \rangle|^2 ,
\]

where the cases \( m_1 = m_2 \) are excluded from the summation. The first term on the right hand side is identical to the expression obtained from \( P_s \) in the case of a single marked state.

We will now show that \( P_s \) for two marked states is the same up to small corrections. To this end we will put an upper bound on the value of the second term in Eq. (56), using the inequality

\[
|\langle m_1 | - \langle m_2 | \phi \rangle|^2 \leq 2 |\langle m_1 | \phi \rangle|^2 + 2 |\langle m_2 | \phi \rangle|^2.
\]

The double summation in the second term of Eq. (56) gives rise to sums of the form \( \sum_{i=0}^{N-1} |\langle i | \phi \rangle|^2 = 1 \). The contribution of this term is found to be just a correction of order \( 1/N \). We thus conclude that the probability of success \( P_s \) of the quantum search algorithm with the initial state \( |\phi \rangle \) and two marked states is identical to Eq. (47), namely, it is the same probability as for a single marked state.

The result of this Section can be easily generalized to the case of \( r \) marked states. In this case the second term on the right hand side of Eq. (56) includes a sum over all the pairs of marked states. The conclusion that \( P_s \) is independent of the number of marked states holds as long as \( r \ll N \).

### G. Calculation of \( P_s \) for certain pure initial states

Consider a state \( |\phi \rangle \) with amplitudes \( a_i \). Since the amplitudes \( a_i = |a_i|e^{i\theta_i}, i = 0, \ldots, N-1 \) are complex numbers and satisfy the normalization condition, the value of \( |\bar{a}| \) increases as the amplitudes become more alligned in the complex plane, namely exhibit a narrow distribution of phases \( \theta_i \), as well as a narrow distribution of the \( |a_i| \)'s. As the distributions become broader the success probability decreases.

For the state \( |\eta \rangle \), in which all the amplitudes are identical, with \( \bar{a} = 1/\sqrt{N} \), the success probability is \( P_s = 1 \). Consider a state \( |\phi \rangle \) in which the amplitudes of \( k \) of the basis states are \( a_i = 1/\sqrt{k} \), and for all the rest \( N - k \) basis states \( a_i = 0 \). For such states the average
amplitude is $\bar{a} = \sqrt{k/N}$ and thus $P_s = k/N$. Clearly, the success probability increases as the amplitude is divided more evenly between the basis states. There are several well known quantum states that can now be examined. One of them is the generalized GHZ state of $n$ qubits

$$|\phi\rangle_{GHZ} = \frac{1}{\sqrt{2}}(|00\ldots0\rangle + |11\ldots1\rangle).$$

(58)

In this state only two of the amplitudes are non-zero. Therefore the success probability $P_s = 2/N \to 0$, as the number of qubits increases. A similar situation is encountered for the $W$ state of $n$ qubits given by

$$|\phi\rangle_W = \frac{1}{\sqrt{n}}(|10\ldots0\rangle + |010\ldots0\rangle + \cdots + |00\ldots1\rangle).$$

(59)

For this state $P_s = n/N$, which also decays to zero as $n$ is increased.

A large class of states for which $P_s$ vanishes up to $O(1/\sqrt{N})$ includes all the states for which $\bar{a} = 0$. This class includes, for example, states in which for each amplitude $a_i$ of basis state $i$, there is a state $j$, with $a_j = -a_i$. In general, a random sampling of states in the Hilbert space of $n$ qubits tends to yield states with very small $\bar{a} \simeq 1/N$. This indicates that generic quantum states of $n$ qubits are highly inefficient as initial states for Grover’s algorithm.

IV. DISCUSSION

Recently it was shown that the success probability of Grover’s algorithm can be used in the construction of an entanglement monotone that quantifies the entanglement of pure quantum states of multiple qubits [23]. To quantify the entanglement of the state $|\phi\rangle$, one is allowed to perform any set of local unitary operations $U_1, U_2, \ldots, U_n$ on the $n$ qubits before feeding the register into the Grover apparatus. These operations are designed to maximize the success probability $P_s$ of the algorithm. For the case of a single marked state, the resulting success probability will thus be [23]

$$P_{\text{max}} = \max_{U_1,\ldots,U_n} \frac{1}{N} \sum_{m_1=0}^{N-1} |\langle m_1 | U^*_G U_1 \otimes U_2 \otimes \cdots \otimes U_n |\phi\rangle|^2 + O \left( \frac{1}{\sqrt{N}} \right),$$

(60)
where the summation takes care of the averaging over all possible choices of the marked state $|m_1\rangle$ and the maximization is over all possible sets of local unitary operators $U_i$, $i = 1, \ldots, n$. It was shown that $P_{\text{max}}$ can be reduced to the form

$$P_{\text{max}} = \max_{|s_1, \ldots, s_n\rangle} |\langle s_1, \ldots, s_n | \phi \rangle|^2 + O\left(\frac{1}{\sqrt{N}}\right),$$

(61)

where the maximization now runs over all product states, $|s_1, \ldots, s_n\rangle = |s_1\rangle \otimes \cdots \otimes |s_n\rangle$, of the $n$ qubits. The maximal success probability is thus determined by the maximal overlap between $|\phi\rangle$ and any product state of $n$ qubits. The Groverian entanglement measure was defined as

$$G(\phi) = \sqrt{1 - P_{\text{max}}}.\quad (62)$$

It was shown that $G(\phi)$ is an entanglement monotone $[23, 25]$. This means that for product states $G(\phi) = 0$, while for any state $|\phi\rangle$ of $n$ qubits it is invariant under any local unitary operations on single qubits. Moreover, $G(\phi)$ cannot be increased by any local operations on the $n$ qubits (where classical communication is allowed between the parties that perform these operations).

The result presented above, that the success probability $P_s$ does not depend on the number of marked states, provides a generalization of the Groverian entanglement. It removes the restriction that $G(\phi)$ will be defined by a search with a single marked state. The use of the Groverian entanglement measure to characterize entangled quantum states of multiple qubits may provide useful insight about the nature of these states and their role in quantum algorithms. To this end one needs to develop efficient computational schemes for the maximization over all possible sets of local unitary operations $U_i$, $i = 1, \ldots, n$ [Eq. (60)], or, alternatively, over all sets of product states [Eq. (61)].

V. SUMMARY

We have analyzed the dynamics of Grover’s quantum search algorithm for the case in which the initial state is an arbitrary pure quantum state $|\phi\rangle$ of $n$ qubits. We have shown that the optimal time to perform the measurement that concludes the operation of the algorithm is independent of the initial state $|\phi\rangle$. It is identical to the optimal measurement time of the original algorithm, with the same number of marked states, in which $|\phi\rangle = |0\rangle$. 

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An expression for the probability of success $P_s$ in terms of the amplitudes of the state $|\phi\rangle$ is obtained and is shown to be independent of the number of marked states, $r$. The fixed points and cycles of the Grover operator $U_G$ are identified. The relevance of the results in the context of using the success probability as an entanglement measure is discussed. In particular, the Groverian entanglement measure, previously limited to a single marked state, is generalized to the case of several marked states. It is shown that as long as $r \ll N$, $G(\phi)$ is independent of $r$.

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