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Entanglement monotone derived from Grover's algorithm

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This paper demonstrates that how well a state performs as an input to Grover's search algorithm depends critically upon the entanglement present in that state; the more the entanglement, the less well the algorithm performs. More precisely, suppose we take a pure state input, and prior to running the algorithm apply local unitary operations to each qubit in order to maximize the probability $P_{\max}$ that the search algorithm succeeds. We prove that, for pure states, $P_{\max}$ is an *entanglement monotone*, in the sense that $P_{\max}$ can never be decreased by local operations and classical communication.

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I. INTRODUCTION

A celebrated result in quantum information science [1,2] is the discovery of quantum algorithms able to solve problems faster than any known classical algorithm. Three such algorithms are Shor's factoring algorithm [3,4], Grover's search algorithm [5,6], and algorithms for quantum simulation (see, for example, [1], and references therein). However, a satisfactory *general* theory of quantum algorithms is yet to be developed. Such a theory must address the question of what makes quantum computers powerful. No complete answer to this question has been given, to date, but it is generally believed that *quantum entanglement* plays a key role. The purpose of this paper is to connect the success of Grover's search algorithm with the amount of entanglement present in the state input to the algorithm.

In particular, we investigate what physical properties of the initial state of Grover's algorithm limit the effectiveness of the algorithm. We show that there is a sense in which *the more entanglement is present in the initial state, the worse Grover's algorithm performs.* To be more precise, suppose we are given a state $|\psi\rangle$ and the ability to do local unitary operations on $|\psi\rangle$ to maximize the probability $P_{\max}(\psi)$ of a successful run of Grover's algorithm. The main result of this paper is to prove that, up to small corrections, $P_{\max}(\psi)$ is an *entanglement monotone* [7]. That is, if $|\psi\rangle$ may be transformed into $|\phi\rangle$ by local operations and classical communication, then we prove that $P_{\max}(\psi) \leqslant P_{\max}(\phi)$, again, up to small corrections. We utilize this observation to construct an entanglement measure, the *Groverian entanglement* of a pure state ψ, $G(\psi)$. We prove that the Groverian entanglement is, up to small corrections, an entanglement monotone, and is equivalent to an entanglement measure proposed previously by Vedral, Plenio, Rippin, and Knight [8]. Thus, this work provides an *operational interpretation* for a multiparty entanglement measure, explicitly connecting that measure to the success probability of a quantum algorithm.

The paper is organized as follows. In Sec. II we describe the quantum search algorithm and derive an exact expression for the maximal success probability for a given initial register state. Motivated by this expression, in Sec. III we introduce the Groverian entanglement, analyze its properties, and show that it is an entanglement monotone. Section IV investigates generalizations of our results to the case of nonqubit systems, to mixed states, and specializes to the case of bipartite systems. Finally, Sec. V summarizes and discusses our results, and suggests directions for further research.

II. THE QUANTUM SEARCH ALGORITHM

In this section we review Grover's quantum search algorithm, and derive an analytic expression for the probability that the algorithm succeeds when the initial input state is an arbitrary pure state of n qubits.

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 their 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 to 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.

Suppose we wish to search the space D to find a marked element. Phrased in terms of the function f, the search for a marked element becomes a search for an element such that $f=1$. 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, $\Theta(N)$ evaluations of f are required on a classical computer. It is one of the most surprising results in quantum information science that, if we allow the function f to be evaluated *coherently*, there exists a sequence of unitary operations which can locate the marked elements using only $O(\sqrt{N/r})$ coherent queries of f [5,6]. This sequence of unitary operations is called Grover's quantum search algorithm.

To describe the operation of the quantum search algorithm we first introduce a register, $|x\rangle=|x_1\ldots x_n\rangle$, of n qubits, and an *ancilla* qubit, $|q\rangle$, to be used in the computation. It will be convenient to sometimes use the label "q" for the ancilla. 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. (For more details on how an oracle may be constructed, see Chap. 6 of [1].) The oracle performs the following unitary operation on computational basis states of the register, $|x\rangle$, and of the ancilla, $|q\rangle$:

$$O|x\rangle|q\rangle=|x\rangle|q\oplus f(x)\rangle, \tag{1}$$

where $\oplus$ denotes addition modulo 2. This definition may be uniquely extended, via linearity, to all states of the register and ancilla.

The oracle recognizes marked states in the sense that if $|x\rangle$ is a marked element of the search space, $f(x)=1$, the oracle flips the ancilla qubit from $|0\rangle$ to $|1\rangle$ and vice versa, while for unmarked states the ancilla is unchanged. In Grover's algorithm the ancilla qubit is initially set to the state $(|0>-|1>)/\sqrt{2}$. It is easy to verify that, with this choice, the action of the oracle is

$$O|x\rangle\left(\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right)=(-1)^{f(x)}|x\rangle\left(\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right). \tag{2}$$

Thus, the only effect of the oracle is to apply a phase of -1 if x is a marked state, and no phase change if x is unmarked. Since the state of the ancilla does not change, it is conventional to omit it, and write the action of the oracle as $O|x\rangle=(-1)^{f(x)}|x\rangle$. Grover's search algorithm may be summarized as follows.

Algorithm 1. Grover's quantum search algorithm.

Inputs. (i) A black box oracle O, whose action is defined by Eq. (1); (ii) $n+1$ qubits in the state $|0\rangle^{\otimes n}|0\rangle_q$.

Outputs. A candidate for a marked state, $|s\rangle$.

Procedure.

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

$$\frac{1}{\sqrt{N}}\sum_{x=0}^{2^n-1}|x\rangle\left(\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right)_q. \tag{3}$$

(2) *Grover iterations*. Repeat the following operation m times, where m is an integer whose construction we describe below.

(a) Apply the oracle, which has the effect of rotating the marked states by a phase of π rad. Since the ancilla is always in the state $(|0\rangle-|1\rangle)/\sqrt{2}$ the effect of this operation may be described by a unitary operator acting only on the register, $I_f^\pi=\Sigma_x(-1)^{f(x)}|x\rangle\langle x|$.

(b) Rotate all register states by π rad around the average amplitude of the register state. This is done by (i) applying the Hadamard gate to each qubit in the register; (ii) rotating the $|00\ldots0\rangle$ state of the register by a phase of π rad. This rotation is similar to 2(a), except for the fact that here it is performed on a known state. It takes the form $I_0^\pi=-|0\rangle\langle 0|+\Sigma_{x\neq 0}|x\rangle\langle x|$. (iii) Again applying the Hadamard gate to each qubit in the register.

The combined operation on the register 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.

Missing from this description is a value for m. As subsequent Grover iterations are applied, the amplitudes of the marked states gradually increase, while the amplitudes of the unmarked states decrease. There exists an optimal number m of iterations at which the amplitude of the marked states reaches a maximum value, and thus the probability that the measurement yields a marked state is maximal. Let us denote this probability by P. It has been shown [6,9] that m is bounded above

$$m\leqslant\left\lceil\frac{\pi}{4}\sqrt{\frac{N}{r}}\right\rceil, \tag{4}$$

where r is the number of marked states and $\lceil x\rceil$ is the smallest integer which is larger than x. The exact value of m as a function of N and r has been constructed in [9,10]. Moreover, it has been shown that Grover's algorithm is optimal in the sense that it is as efficient as theoretically possible [11], and that it is possible to obtain the marked state with very high probability, $P=1-O(1/\sqrt{N})$, after m iterations [9,10]. Note that $P\approx 1$ only occurs for the specific starting state described in step 1 of Algorithm 1, above. If the Grover iterations start from an arbitrary state, then P may be bounded away from 1 [12].

In this paper we are interested in determining what properties of the initial state of the register are responsible for the efficiency of the quantum search algorithm. To this end, we propose modifying the initialization step, as described by the following hypothetical situation. Consider n parties (Alice, Bob, Charlie, ..., Narelle) sharing a pure quantum state $|\phi\rangle$. For simplicity, we initially assume that $|\phi\rangle$ is a state of n qubits, and each party is in possession of one qubit. The parties wish to cooperate in a joint venture in which they use *those particular n qubits* to perform a quantum search of the space of $N=2^n$ elements. The parties are unable to employ any communication channels. Prior to the search, each party may perform local unitary operations on the qubit in their possession. After they complete the local processing of their qubits, all parties send (or teleport) their qubits to the search processing unit. The only processing available in this unit is Grover's search iterations and the subsequent measurement. Thus, the only way the qubits are allowed to interact is through Grover iterations.

This modified quantum search algorithm, which, with variations, we study for the remainder of this paper, may be summarized as follows.

Algorithm 2. Modified quantum search.

Inputs. (i) A black box oracle O, whose action is defined by Eq. (1); (ii) $n+1$ qubits in the state $|\phi\rangle|0\rangle_q$.

Outputs. A candidate for a marked state, $|s\rangle$.

Procedure.

(1) *Initialization*. Apply to the input register-ancilla state, $|\phi\rangle|0\rangle_q$, a product of arbitrary local operations on the register, $V=U_1\otimes U_2\otimes\cdots\otimes U_n$, and the gate HX on the ancilla, where U_j is an arbitrary local unitary gate acting on the jth qubit. The resulting state is

$$|\psi\rangle\otimes\left(\frac{|0\rangle-|1\rangle}{\sqrt{2}}\right)_q=V|\phi\rangle\otimes HX|0\rangle_q. \tag{5}$$

(2) *Grover iterations*. Repeat the following operation m times, where m is chosen as described above.

(a) Rotate the marked states by a phase of π rad, as in Algorithm 1.

(b) Rotate all register states by π rad around the average amplitude of the register state, as in Algorithm 1.

The combined operation on the register 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.

This modification of Grover's algorithm may appear somewhat *ad hoc*. However, as we now explain, the modification allows a connection between Grover's algorithm and measures of entanglement to be made.

The connection follows by asking what is the maximal probability of success, $P_{\max}$, that a marked element is found, where the maximization is over all possible local unitary operations in the initialization step? We will analyze this question for the case where there is just a *single* marked solution, which we denote s, to the search problem. We show that in this case $P_{\max}$ is related to the entanglement present in the initial register state, $|\phi\rangle$.

To make this assertion more precise, let us write $P_{\max}$ in terms of the operator U_G^m representing m Grover iterations. Averaging uniformly over all N possible values for s [13] we see that this probability may be written

$$P_{\max}=\max_{U_1,\ldots,U_n}\frac{1}{N}\sum_{s=0}^{N-1}|\langle s|U_G^m(U_1\otimes U_2\otimes\cdots\otimes U_n)|\phi\rangle|^2, \tag{6}$$

where the maximization is over all local unitary operations $U_1,\ldots,U_n$ on the respective qubits.

To analyze Eq. (6) for a general state, $|\phi\rangle$ a simple trick allows us consider only the action of the Grover iterations on the equal superposition state $|\eta\rangle=\Sigma_x|x\rangle/\sqrt{N}$, which is usually used as the input to Grover's algorithm. Applying m Grover iterates to this state yields

$$U_G^m|\eta>=|s\rangle+O\left(\frac{1}{\sqrt{N}}\right), \tag{7}$$

where the second term is a small correction due to the fact that Grover's algorithm does not yield a solution with probability 1, but rather with probability $1-O(1/\sqrt{N})$. Multiplying this equation by $(U_G^m)^\dagger$ and then taking the Hermitian conjugate gives

$$\langle s|U_G^m=\langle\eta|+O\left(\frac{1}{\sqrt{N}}\right). \tag{8}$$

Substituting into Eq. (6) gives, for a general state $|\phi\rangle$,

$$P_{\max}=\max_{U_1,\ldots,U_n}\frac{1}{N}\sum_{s=0}^{N-1}|\langle\eta|U_1\otimes U_2\otimes\cdots\otimes U_n|\phi\rangle|^2+O\left(\frac{1}{\sqrt{N}}\right). \tag{9}$$

However, $|\eta\rangle$ is a product state, so that $U_1^\dagger\otimes U_2^\dagger\otimes\cdots\otimes U_n^\dagger|\eta\rangle$ is another product state. Therefore, the optimization in Eq. (9) may, equivalently, be expressed as an optimization over product states,

$$P_{\max}=\max_{|e_1,\ldots,e_n\rangle}|\langle e_1,\ldots,e_n|\phi\rangle|^2+O\left(\frac{1}{\sqrt{N}}\right), \tag{10}$$

where the maximization now runs over all product states, $|e_1,\ldots,e_n\rangle=|e_1\rangle\otimes\cdots|e_n\rangle$, of the n qubits. In order for the parties Alice, Bob, Charlie, . . . , Narelle to achieve this maximum probability when running Algorithm 2, they apply to the joint state $|\phi\rangle$ local unitary rotations U_j which have the effect of taking $|e_j\rangle$ to $(|0\rangle+|1\rangle)/\sqrt{2}$.

This expression, Eq. (10), takes a suggestive form. Up to corrections of order $1/\sqrt{N}$ it depends monotonically on the maximum of the overlap between all product states and the input state $|\phi\rangle$ [14]. If the input state were a product, $|\phi\rangle=|u_1\rangle\otimes|u_2\rangle\otimes\cdots\otimes|u_n\rangle$, then $P_{\max}$ would be equal to 1, again, up to small corrections. If, alternatively, the input state were not a product state, it would never be possible for the modified search algorithm to succeed with probability 1. These observations suggest that $P_{\max}$ depends, in some way, on the entanglement of the initial register state, $|\phi\rangle$.

III. AN ENTANGLEMENT MEASURE FROM THE QUANTUM SEARCH ALGORITHM

In the preceding section we suggested that the maximum success probability, $P_{\max}$, of Algorithm 2, depended on the entanglement of the initial state of the register. In this section, we show that $P_{\max}$ can be used to define an entanglement measure, the *Groverian entanglement*, for arbitrary pure multiple qubit states. We show that the Groverian entanglement is closely related to an entanglement measure introduced previously by Vedral, Plenio, Rippin, and Knight [8] (see also Vedral and Plenio [15], and Barnum and Linden [16]). This connection enables us to understand some properties of the Groverian entanglement making it a good entanglement measure.

Before defining the Groverian entanglement, we briefly overview some common approaches taken to the definition of entanglement measures. Broadly speaking, there are two main approaches, an *operational approach*, and an *axiomatic* approach. In the operational approach [17], the measures of entanglement are related to physical tasks that one can perform with a quantum state, as quantum communication. The axiomatic approach (see, for example, [7,8]) starts from desirable axioms that a "good" entanglement measure should satisfy, and then attempts to construct such measures.

The Groverian entanglement is an example of an entanglement measure defined in operational terms, namely, how well a state serves as the input to Algorithm 2. We define the Groverian entanglement of a state $|\psi\rangle$ by

$$G(\psi)\equiv\sqrt{1-P_{\max}}. \tag{11}$$

Note that we will freely interchange the notations $|\psi\rangle$ and ψ. Since $P_{\max}$ takes values in the range $0\leqslant P_{\max}\leqslant 1$, it follows that $0\leqslant G(\psi)\leqslant 1$. However, it is not immediately clear that $G(\psi)$ is a good measure of entanglement. We show that this is the case by using the results of the preceding section to connect $G(\psi)$ to a measure of entanglement introduced in [8], following the axiomatic approach.

To demonstrate the connection between the Groverian entanglement and [8], we substitute Eq. (10) into Eq. (11), and move the maximization outside the square root, where it becomes a minimization. Neglecting terms of $O(1/\sqrt{N})$ this gives

$$G(\psi)=\min_{|e_1,\ldots,e_n\rangle}\sqrt{1-F^2(e_1\otimes\cdots\otimes e_n,\psi)}, \tag{12}$$

where $F(\cdot,\cdot)$ is the *fidelity* [1,18,19], defined in general by $F(\rho,\sigma)\equiv\mathrm{tr}(\sqrt{\rho}\sigma\sqrt{\rho})^{1/2}$. Special cases of interest are the pure state fidelity, $F(a,b)=|\langle a|b\rangle|$, and the case where one state is pure and one state is mixed, $F(\sigma,a)=\langle a|\sigma|a\rangle^{1/2}$. We now show that we can extend the range of the minimization in Eq. (12) to a minimization over the space $\mathcal{S}$ of *all* separable density matrices, that is, density matrices which can be written in the form $\sigma=\Sigma_j p_j\rho_j^1\otimes\cdots\otimes\rho_j^n$,

$$G(\psi)=\min_{\sigma\in\mathcal{S}}\sqrt{1-F^2(\sigma,\psi)}. \tag{13}$$

To see this, simply note that by linearity of $F^2(\sigma,\psi)$ in σ, and convexity of $\mathcal{S}$, the maximal value of $F^2(\sigma,\psi)$, and thus the minimum in $\sqrt{1-F^2(\sigma,\psi)}$, can always be obtained at an extreme point of $\mathcal{S}$, that is, when σ is a pure product state.

The expression Eq. (13) for the Groverian entanglement should be compared with the following definition of an entanglement measure, introduced in [8] by Vedral, Plenio, Rippin, and Knight [20]:

$$E(\psi)\equiv 2-2\max_{\sigma\in\mathcal{S}}F(\sigma,\psi). \tag{14}$$

This definition is essentially equivalent to ours, in that $G(\psi)$ is a monotonic function of $E(\psi)$, and vice versa. Vedral *et al.* introduced their definition motivated primarily by axiomatic concerns; we have shown that, in fact, there is a close connection between this measure and the utility of the state as an input to Grover's algorithm.

We now briefly describe several useful properties of the Groverian entanglement. The proofs are the same as those given in [8] (see also [15,16]); what is different is the connection between this measure of entanglement and Grover's algorithm. It is clear that $G(\psi)=0$ iff $|\psi\rangle$ is a product state, and that local unitary operations on the qubits leave $G(\psi)$ invariant. What is more surprising in the context of Grover's algorithm, and is the main result of this paper, is that $G(\psi)$ is an *entanglement monotone*. That is, $G(\psi)$ cannot be increased by local operations and classical communication:

Theorem. Let $|\psi\rangle$ and $|\phi\rangle$ be n-qubit pure states such that it is possible to transform $|\psi\rangle$ to $|\phi\rangle$ by local operations on the qubits, and classical communication. Then $G(\psi)\geqslant G(\phi)$, up to corrections of order $1/\sqrt{N}$.

This theorem has the remarkable implication that the probability $P_{\max}$ of success for our modified Grover's algorithm can *never decrease* under local operations and classical communication. The proof of the theorem follows easily by rewriting Eq. (13) in terms of the metric defined by [21]

$$B(\rho,\sigma)\equiv\sqrt{1-F^2(\rho,\sigma)}, \tag{15}$$

which results in

$$G(\psi)=\min_{\sigma\in\mathcal{S}}B(\sigma,\psi). \tag{16}$$

Suppose $|\psi\rangle$ can be transformed into $|\phi\rangle$ by a process of local operations and classical communication, whose effect is represented by the quantum operation [1] $\mathcal{E}$. Let σ be the state for which the minimum in Eq. (16) is achieved, $G(\psi)=B(\sigma,\psi)$. It can be shown [22] that the distance $B(\rho,\sigma)$ between two states can never be increased by a quantum operation, so

$$G(\psi)=B(\sigma,\psi) \tag{17}$$

$$\geqslant B(\mathcal{E}(\sigma),\mathcal{E}(|\psi\rangle\langle\psi|)) \tag{18}$$

$$=B(\mathcal{E}(\sigma),\phi). \tag{19}$$

But σ is separable, so $\mathcal{E}(\sigma)$ is also separable, since it can be obtained by local operations and classical communication from σ. Thus

$$G(\psi)\geqslant B(\mathcal{E}(\sigma),\phi)\geqslant G(\phi), \tag{20}$$

which completes the proof that $G(\cdot)$ is an entanglement monotone.

IV. EXTENSIONS OF THE GROVERIAN ENTANGLEMENT

In this section we investigate three scenarios generalizing the earlier results about n-qubit pure state entanglement. Section IV A addresses systems whose subsystems are not qubits but instead have arbitrary (finite) dimensionality. Section IV B specializes to the case of a *bipartite* quantum system, where the two subsystems have arbitrary finite dimensionalities. Finally, in Sec. IV C we consider whether the Groverian entanglement is a good measure of entanglement for mixed states.

A. Groverian entanglement for subsystems of arbitrary dimensionality

As described earlier, Algorithm 2 is applied to a system of n qubits, and thus the Groverian entanglement is only defined for such a system. However, with a small modification the algorithm we described can be extended to the case of n systems of arbitrary finite dimensionalities, $d_1, d_2, \ldots, d_n$.

The only change is in the inversion about the average, step 2(b). To achieve the analogous operation, we need to find a replacement for the Hadamard gate. Suppose V_j is any $d_j \times d_j$ unitary operator such that $V_j|0\rangle = \Sigma_{k=0}^{d_j-1}|k\rangle/\sqrt{d_j}$, where $|0\rangle, \ldots, |d_j-1\rangle$ forms an orthonormal basis for the state of the jth system. For example, V_j could be the matrix representation of the Fourier transform over the integers modulo d_j. Then the inversion about the average can be achieved by (i) applying the operation V_j to each system; (ii) rotating the $|00\ldots0\rangle$ state of the register by a phase of π rad. This rotation takes the form $I_0^\pi = -|0\rangle\langle 0| + \Sigma_{x\neq 0}|x\rangle\langle x|$; (iii) applying the inverse operation $V_j^{\dagger ger}$ to each system.

With this modification, the Grover iterate can be used to perform quantum searches using systems of arbitrary dimensionality. Proceeding as before, we find that Eq. (10) holds even for systems of arbitrary dimensionality, that is,

$$P_{\max} = \max_{|e_1,\ldots,e_n\rangle} |\langle e_1,\ldots,e_n|\phi\rangle|^2 + O\left(\frac{1}{\sqrt{N}}\right). \tag{21}$$

Similarly, if we define the Groverian entanglement by $G(\psi) \equiv \sqrt{1-P_{\max}}$ then the same argument as before shows that the Groverian entanglement is an entanglement monotone, up to corrections of $O(1/\sqrt{N})$, and can thus be regarded as a good measure of entanglement for composite systems of arbitary dimensionality.

B. Two-party Groverian entanglement

In this section we specialize our study of the Groverian entanglement to bipartite quantum systems and derive an analytic expression for the Groverian entanglement in that case. We suppose that the two-component systems have arbitrary finite dimensionalities, d_1 and d_2. In the bipartite case the optimization in Eq. (21) is equivalent to the maximization of the fidelity

$$F(U\otimes V|0\rangle_A|0\rangle_B, \phi), \tag{22}$$

where we use the fact that any product state may be written as a product of two local unitaries operating on some fiducial state $|0\rangle_A|0\rangle_B$. This problem has been considered in [23,24], where it was shown that the solution may be obtained in terms of the *Schmidt decomposition* [1] of $|\phi\rangle$,

$$|\phi\rangle = \sum_i \sqrt{p_i}|u^i\rangle_A|v^i\rangle_B, \tag{23}$$

where $|u^i\rangle$ and $|v^i\rangle$ are each orthonormal sets of vectors, and the Schmidt coefficients $\sqrt{p_i}$ are non-negative real numbers. [23,24] showed that the maximum occurs when $U\otimes V|0\rangle_A|0\rangle_B = |u^i\rangle_A|v^i\rangle_B$ where i is chosen so that $\sqrt{p_i} = \sqrt{p_{\max}}$ is the maximal Schmidt coefficient. Substituting into Eq. (21) gives

$$G(\psi) = \sqrt{1-p_{\max}}. \tag{24}$$

Thus, for a bipartite system the Groverian entanglement is equivalent to a well-known entanglement monotone [7,25], the square of the largest Schmidt coefficient. Indeed, for the case of two qubits, $G(\psi)$ is equivalent to the usual asymptotic measure of pure state entanglement [17,26,27], the von Neumann entropy of the reduced density operator for either qubit, $S = -\mathrm{tr}(\rho_A \ln \rho_A)$. The relationship between the two quantities is $S = h(G^2(\psi))$, where $h(x) = -x\log_2 x - (1-x)\log_2(1-x)$ is the binary entropy.

C. The Groverian entanglement for mixed states

We have defined the Groverian entanglement and investigated its properties for the special case of pure state inputs to Grover's algorithm. How does the analogous measure behave for mixed states? Is it still a good measure of entanglement? In this section we briefly consider these questions. We show that the natural generalization to mixed states is not a good measure of entanglement, and discuss other possible ways of generalizing the Groverian entanglement to mixed states.

Suppose a mixed state ρ is used as the input in Algorithm 2, replacing the pure state $|\phi\rangle$. Then it is not difficult to show that the corresponding maximal probablity of success is given by

$$P_{\max} = \max_{|e_1,\ldots,e_n\rangle} \langle e_1,\ldots,e_n|\rho|e_1,\ldots,e_n\rangle + O\left(\frac{1}{\sqrt{N}}\right), \tag{25}$$

which is the linear extension of the expression in Eq. (10) to a general density matrix. Suppose we define

$$G(\rho) \equiv \sqrt{1-P_{\max}}. \tag{26}$$

For pure states this agrees with the earlier definition of the Groverian entanglement.

Suppose $\rho = \rho_1 \otimes \cdots \otimes \rho_n$, and that λ_j is the largest eigenvalue of ρ_j. Then from Eq. (25), $P_{\max} = \lambda_1\lambda_2\cdots\lambda_n$, and thus

$$G(\rho_1\otimes\cdots\otimes\rho_n) = \sqrt{1-\prod_{j=1}^n \lambda_j}. \tag{27}$$

In the case when $\rho_1, \ldots, \rho_n$ are pure states, all the $\lambda_j = 1$, and $G(\rho) = 0$. However, when the ρ_j are mixed, the values of $G(\rho)$ may span the entire range from $G(\rho)$'s minimal value of 0, right up to its maximal possible value of $\sqrt{1-1/N}$. It follows that $G(\rho)$ cannot be an entanglement monotone.

From these observations we conclude that $G(\rho)$ is not a good measure of entanglement for mixed states. The essential problem is that $G(\rho)$ is linear in ρ, and many states that we ordinarily think of as not being entangled can be represented as a mixture of entangled states. For example, the completely mixed state $I\otimes I/4$ of two qubits can be written as an equal mixture of maximally entangled states. By linearity, $G(I\otimes I/4)$ therefore takes the same value as for a maximally entangled state.

Is there any sensible way of resolving this difficulty with mixed states? At present, we are not aware of any natural resolution that preserves the elegant operational interpretation of the Groverian entanglement. It is interesting to note, however, that the measure of entanglement proposed by Vedral *et al.* [8] applied equally well to either pure or mixed states. In particular, for a general mixed state ρ of a composite system one can define

$$\tilde{G}(\rho) \equiv \min_{\sigma \in \mathcal{S}} \sqrt{1 - F^2(\rho,\sigma)}, \tag{28}$$

where the minimization is over all *separable* states σ of the system, and $F(\rho,\sigma)$ is the fidelity, as defined earlier. This is a generalization of our measure for pure states, however we have not succeeded in obtaining a good operational interpretation of $\tilde{G}(\rho)$ along lines similar to the pure state case. Another possible resolution, following a line of thought similar to [16], is to define

$$\hat{G}(\rho) \equiv \min \sum_j p_j G(\psi_j), \tag{29}$$

where the minimum is over all ensembles $\{p_j, |\psi_j\rangle\}$ such that $\rho = \Sigma_j p_j |\psi_j\rangle\langle\psi_j|$. It is not difficult to show that $\hat{G}(\rho)$ is an entanglement monotone, locally unitarily invariant, and is equal to zero if and only if ρ is separable. However, once again, a good operational interpretation of $\hat{G}(\rho)$ is presently unknown to us.

V. SUMMARY, DISCUSSION, AND FUTURE DIRECTIONS

In this paper we have investigated the relationship between the success probability of a modified form of Grover's quantum search algorithm, and the amount of entanglement present in the initial state used for the algorithm. We have proposed an entanglement measure for n-party pure states, the Groverian entanglement, based on the maximal success probability of the algorithm. Furthermore, we showed that the Groverian entanglement is essentially equivalent to a measure of entanglement introduced by Vedral, Plenio, Rippin and Knight [8], and used this to argue that the Groverian entanglement and $P_{\max}$ are entanglement monotones.

The interpretation of Grover's algorithm we have developed in this paper should be compared with that obtained by Miyake and Wadati in their recent paper [28]. In [28] it was shown that the progress of the unmodified Grover's algorithm corresponds to a traversal of a geodesic (or shortest path) in the complex projective Hilbert space geometry of all states, where the metric is taken to be the Fubini-study metric. These results are, in a sense, dual to the results we have obtained in this paper. We have managed to show that, given the additional freedom to apply local unitaries to an arbitrary input, Grover's algorithm not only correponds to a traversal of the shortest path between the initial state and target state (thus complementing the results of [28]), but also that its success probability depends on the entanglement content of the initial state in a monotone fashion.

Our work suggests several directions for future research. It would be interesting to investigate other variants of Grover's algorithm, including the following.

(1) Allowing multiple solutions in the search space, rather than a single solution, as we have considered.

(2) Replacing the two Hadamard transforms in the Grover iterate by an arbitrary unitary transform U and its inverse $U^\dagger$, respectively.

(3) Tracking the evolution of the entanglement present in intermediate stages of the algorithm. Investigations along these lines, but in a somewhat different context, have been reported in [29–31].

(4) Determining the effect noise has on the performance of the algorithm, and entanglement measures derived from the algorithm.

It would also be interesting to investigate other quantum algorithms, such as Shor's algorithm, quantum simulation, and adiabatic quantum computation [32]. We hope that by pursuing such investigations, insight will be obtained into the fundamental question of what makes quantum computers powerful. Also it will elucidate the role entanglement plays in quantum information processing.

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[14] The correction term in Eq. (7) may actually be removed by an additional modification of Grover's algorithm in which the rotations in the Grover iterate are not by π rad, but rather by some other angle close to π. For the sake of clarity we do not concern ourselves with this issue, and will mostly be content to ignore the corrections of order $1/\sqrt{N}$ in any case.

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[21] The fact that this is a metric follows easily from Uhlmann's theorem [18] that $F(\rho,\sigma)=\max_{\psi,\phi}|\langle\psi|\phi\rangle|$, where ψ and ϕ are purifications of ρ and σ, and the easily verified fact that for pure states ψ and ϕ, $\mathrm{tr}||\psi\rangle\langle\psi|-|\phi\rangle\langle\phi||/2=\sqrt{1-|\langle\psi|\phi\rangle|^2}$ is a metric on pure states, and thus satisfies the triangle inequality.

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