Spatial Search by Quantum Walk is Optimal for Almost all Graphs

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The problem of finding a marked node in a graph can be solved by the spatial search algorithm based on continuous-time quantum walks (CTQW). However, this algorithm is known to run in optimal time only for a handful of graphs. In this work, we prove that for Erdös-Renyi random graphs, i.e., graphs of $n$ vertices where each edge exists with probability $p$, search by CTQW is almost surely optimal as long as $p \geq \log^{3/2}(n)/n$. Consequently, we show that spatial search is in fact optimal for almost all graphs, meaning that the fraction of graphs of $n$ vertices for which this optimality holds tends to one in the asymptotic limit. We obtain this result by proving that search is optimal on graphs where the ratio between the second largest and the largest eigenvalue is bounded by a constant smaller than 1. Finally, we show that we can extend our results on search to establish high fidelity quantum communication between two arbitrary nodes of a random network of interacting qubits, namely, to perform quantum state transfer, as well as entanglement generation. Our work shows that quantum information tasks typically designed for structured systems retain performance in very disordered structures.

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Quantum walks provide a natural framework for tackling the spatial search problem of finding a marked node in a graph of $n$ vertices. In the original work of Childs and Goldstone [1], it was shown that continuous-time quantum walks can search on complete graphs, hypercubes, and lattices of dimensions larger than four in $O(\sqrt{n})$ time, which is optimal. More recently, new instances of graphs have been found where the spatial search works optimally. These examples show that global symmetry, regularity, and high connectivity are not necessary for the optimality of the algorithm [2–4]. However, it is not known how general the class of graphs is for which the spatial search by quantum walk is optimal. Here we address the following question: If one picks at random a graph from the set of all graphs of $n$ nodes, can one find a marked node in optimal time using quantum walks? We show that the answer is almost surely yes. Moreover, we adapt the spatial search algorithm to protocols, for state transfer and entanglement generation between arbitrary nodes of a network of interacting qubits, that work with high fidelity for almost all graphs, for large $n$ (nodes and vertices are used interchangeably throughout the Letter). Thus, besides showing that spatial search by quantum walk is optimal in a very general scenario, we also show that other important quantum information tasks, typically designed for ordered systems, can be accomplished efficiently in very disordered structures.

We obtain our results by studying the spatial search problem in Erdös-Renyi random graphs, i.e., graphs of $n$ vertices where an edge between any two vertices exists with probability $p$ independently of all other edges, typically denoted as $G(n, p)$ [5,6]. Note that our approach is different from the quantum random networks of noninteracting qubits defined in Ref. [7], where two nodes are connected if they share a maximally entangled state, having in view long-distance quantum communication. Also, in Refs. [8,9], the authors compare the dynamics of classical and quantum walks on Erdös-Renyi graphs and other complex networks, although with a different perspective from our work.

In our work, we show that search is optimal on $G(n, p)$ with probability that tends to one as $n$ tends to infinity, as long as $p \geq \log^{3/2}(n)/n$. It can be demonstrated that when $p = 1/2$, $G(n, 1/2)$ is a graph picked at random from the set of all graphs of $n$ nodes in an unbiased way; i.e., each graph is picked with equal probability. This allows us to conclude that spatial search by quantum walk is optimal for almost all graphs from this set. To obtain this result, we prove a sufficient condition regarding the adjacency matrix of graphs where search is optimal: the eigenstate corresponding to its largest eigenvalue must be sufficiently delocalized and the ratio between the second largest and the largest eigenvalues must be bounded by a constant smaller than 1.

This general result also allows us to prove that search is optimal for graphs sampled uniformly from the set of all regular graphs, also known as random regular graphs. Thus, this leads us to conclude that spatial search by quantum walk is optimal for almost all regular graphs.

A sufficient condition for optimal quantum search.— Let $G$ be a graph with a set of vertices $V = \{1, \ldots, n\}$. We consider the Hilbert space spanned by the localized quantum states at the vertices of the graph $\mathcal{H} = \text{span}\{\ket{1}, \ldots, \ket{n}\}$, and the following search Hamiltonian:

$$H = \sum_{i=1}^{n} \lambda_i \ket{\psi_i} \bra{\psi_i},$$

where $\lambda_i$ are the eigenvalues of the adjacency matrix of $G$ and $\ket{\psi_i}$ are the corresponding eigenvectors. The goal is to find a marked node $m$ in optimal time, i.e., $\text{O}(\sqrt{n})$. This can be achieved by using the quantum walk Hamiltonian $H$ with a squared phase shift $\alpha^2$ applied to the marked node:

$$H' = \sum_{i=1}^{n} (\alpha^2 \delta_{mi} + \lambda_i) \ket{\psi_i} \bra{\psi_i}.$$
where $|w⟩$ corresponds to the solution of the search problem, $γ$ is a real number and $A_G$ is the adjacency matrix of a graph $G$ [1]. We say that quantum search by continuous time quantum walk is optimal on a graph $G$ if there is an initial state $|ψ_0⟩$, irrespective of $w$, and a value of $γ$ such that after a time $T = O(√n)$ [10], the probability of finding the solution upon a measurement in the vertex basis is $|⟨w|e^{-iH_0T}|ψ_0⟩|² = O(1)$. The initial state $|ψ_0⟩$ is usually chosen to be the equal superposition of all vertices, i.e., the state $|s⟩ = \sum_{i=1}^{n} |i⟩/√n$, since it is not biased towards any vertex of the graph. We start by proving the following general lemma regarding the spectral properties of $A_G$ and the optimality of search:

**Lemma 1:** Let $H_1$ be a Hamiltonian with eigenvalues $λ_1 ≥ λ_2 ≥ … ≥ λ_k$ (satisfying $λ_1 = 1$ and $|λ_i| ≤ c < 1$ for all $i > 1$) and eigenvectors $|v_1⟩, |v_2⟩, … , |v_k⟩$ and let $H_2 = |w⟩⟨w| + |w⟩⟨s| = c$. For an appropriate choice of $r = O(1)$, applying the Hamiltonian $(1 + r)H_1 + H_2$ to the starting state $|v_1⟩ = |s⟩$ for time $Θ(1/c)$ results in a state $|f⟩$ with $|⟨w|f⟩|² ≥ (1 - c)/(1 + c) - O(1)$.


Thus, if $λ_1 ≥ λ_2 ≥ … ≥ λ_A$ are the eigenvalues of the adjacency matrix $A_G$, we choose $γ = 1/λ_1$ and, consequently, $H_1 = γA_G$. If $|s⟩$ is an eigenstate of $A_G$ corresponding to its largest eigenvalue $λ_A$, and since $|⟨w|s⟩| = 1/√n$, we have that search is optimal as long as $λ_2/λ_1 ≤ c < 1$, following Lemma 1. We will see that Erdős-Rényi graphs and random regular graphs fulfill this property, leading to the conclusion that search is optimal for almost all graphs and also for almost all regular graphs (the latter is discussed in Sec. II of the Supplemental Material [11]).

In fact, Lemma 1 implies that for any regular graph having a constant normalized algebraic connectivity, quantum search is optimal [14]. This is in contrast to Ref. [4] where two examples of regular graphs [15] with low normalized algebraic connectivity are given, such that quantum search is optimal on one and nonoptimal on the other. This result showed that normalized algebraic connectivity is not a necessary condition for fast quantum search: when connectivity is low, search can be fast or slow depending on the graph. On the other hand, Lemma 1 proves that high connectivity is indeed a sufficient condition.

**Quantum search on Erdős-Rényi random graphs.**— Let us consider a graph $G(n)$ with a set of vertices $V = \{1, … , n\}$. We restrict ourselves to simple graphs, i.e., graphs which do not contain self-loops or multiple edges connecting the same pair of vertices. The maximum number of edges that a simple graph $G(n)$ can have is $N = \binom{n}{2}$. Thus, there are $\binom{N}{M}$ graphs of $M$ edges and the total number of (labeled) graphs is $\sum_{M=0}^{N} \binom{N}{M} = 2^N$ [16].

Now let us consider the random graph model $G(n, p)$, a graph with $n$ vertices where we have an edge between any two vertices with probability $p$, independently of all the other edges [5, 6, 17]. In this model, a graph $G_0$ with $M$ edges appears with probability $P(G(n, p) = G_0) = p^M(1 - p)^{N - M}$. In particular, if we consider the case $p = 1/2$, each of the $2^N$ graphs appears with equal probability $P = 2^{-N}$. In their seminal papers, Erdős and Rényi introduced this model of random graphs and studied the probability of a random graph to possess a certain property $Q$ [5, 6]. They studied properties like connectedness of the graph, the probability that a certain subgraph is present, etc. They introduced the terminology stating that almost all graphs have a property $Q$ if the probability that a random graph $G(n, p)$ has $Q$ goes to 1 as $n → ∞$.

Equivalently, it can be stated that $G(n, p)$ almost surely has property $Q$. Interestingly, certain properties of random graphs arise suddenly for a certain critical probability $p = p_c$, where this probability depends typically on $n$. More precisely, if $p(n)$ grows faster than $p_c(n)$, the probability that the random graph has property $Q$ goes to 1 in the asymptotic limit, whereas if it grows slower than $p_c(n)$ it goes to 0. For example, above the percolation threshold, i.e., when $p > 4\log(n)/n$ the graph is almost surely connected, whereas if $p < 4\log(n)/n$ the graph has almost surely isolated nodes.

In this work, we are interested in the threshold value of $p$ for which quantum search becomes optimal; i.e., a marked vertex from the graph can be found in $O(√n)$ time. We consider the search Hamiltonian in Eq. (1) for Erdős-Rényi random graphs $H_{G(n, p)} = -|w⟩⟨w| - γA_{G(n, p)}$. In order to apply Lemma 1 we need to know the largest eigenvalue of $A_{G(n, p)}$, which we denote as $λ_A$, its corresponding eigenstate $|v_1⟩$ and the second largest eigenvalue of $A_{G(n, p)}$ denoted as $λ_2$. It was shown in Ref. [18] that the highest eigenvalue $λ_A$ is a random variable whose probability distribution converges to a Gaussian distribution with mean $np$ and standard deviation $\sqrt{p(1 - p)}$, as $n → ∞$. The corresponding eigenstate, $|v_1⟩$, tends almost surely to $|s⟩ = 1/√n \sum_{i=1}^{n} |i⟩$. For a more detailed analysis of the convergence of $|v_1⟩$ to $|s⟩$, refer to Lemma 2 in Sec. III of the Supplemental Material [11]. It is also possible to obtain an upper bound on the second highest eigenvalue, $λ_2$ from the results of Ref. [18] which applies to random symmetric matrices. In fact in Ref. [19], a tighter bound on $λ_2$ is provided as $n → ∞$, given by

$$λ_2 = 2√np + O((np)^{1/4} \log(n)).$$

We see that as long as $p ≥ 4\log^{1/3}(n)/n$, the ratio $λ_2/λ_A$ is bounded by a constant. However, as can be seen in Sec. III of Supplemental Material [11], in order to ensure that $|v_1⟩$ converges to $|s⟩$, almost surely, we choose the critical value of $p$ for search to be optimal as $p ≥ 100501/^32(n)/n$. In fact, in the asymptotic limit, $λ_2/λ_A → 0$, and the eigenstates corresponding to the two lowest eigenvalues of $H_{G(n, p)}$ are
than the solution state numerically (in blue) for from Eq. (4) (in red) and the exact solution calculated
from Eq. (4) for the probability of success. When the two lowest
and the rest of the spectrum the better is the prediction from
perturbation theory. We fix the number of vertices
percolation threshold and thus the semicircle law is not valid. We
see that the larger the gap between the two lowest eigenvalues
is close to
1
w
, 0.01, and 0.002 in (a),(b), and (c), respectively. Right
side: Spectrum of the search Hamiltonian for instances of random
graphs that provide the dynamics represented on the left side. In
(c) this does not happen since
p
is close to 1/n, which is the
percolation threshold and thus the semicircle law is not valid. We
see that the larger the gap between the two lowest eigenvalues
and the rest of the spectrum the better is the prediction from
Eq. (4) for the probability of success. When the two lowest
eigenvalues are not isolated, the probability of observing the
solution is low and the algorithm does not provide speed-up with
respect to classical search.

\[ |\lambda_\pm| \approx \left| \frac{w}{\sqrt{2}} \pm \frac{s_w}{\sqrt{2}} \right|, \]

where \( s_w \) is the equal superposition of all the vertices other
than the solution state \( |w\rangle \). The probability of success is

\[ P_w(t) = |\langle w| \exp(-iH_{G(n,p)}t)|s\rangle|^2 = \sin^2 \left( \frac{t}{\sqrt{n}} \right). \]

To confirm these theoretical predictions we plot, on the left
side of Figs. 1(a)–1(c), the approximate probability \( P_w(t) \)
from Eq. (4) (in red) and the exact solution calculated
numerically (in blue) for \( n = 1000 \) and \( p = 0.1, 0.01, \)
0.002. On the right side, we plot the spectrum of the
respective Hamiltonians. We observe, as expected, that
the larger the gap between the two lowest eigenvalues
and the bulk of the spectrum, the better is the approximation
given by Eq. (4) for the probability of success of search. As
this gap disappears, close to the percolation threshold, the
eigenstates corresponding to the two lowest eigenvalues do
not follow Eq. (3) and will mix randomly with the subspace
orthogonal to \(|w\rangle\) and \(|s_w\rangle\). At this point, since we are close
to the percolation threshold, the graph is expected to have
some isolated components and the algorithm breaks [see
Fig. 1(c)].

So far we have made the choice \( \gamma = 1/\lambda_1^A \), and assumed
that we know the value of the random variable \( \lambda_1^A \). In fact,
its standard deviation is small enough so that it is
sufficient to know its mean, which is equal to \( np \), i.e.,
we can choose \( \gamma = 1/(np) \), in order to prove that search is
optimal almost surely. We prove this in Sec. IV of the
Supplemental Material [11], using tools of degenerate
perturbation theory. These tools are also useful to design
protocols for performing optimal state transfer and entan-
glement generation in Erdös-Renyi graphs, as will be
explained subsequently.

**State transfer with high fidelity.**—Quantum state transfer
in spin chains [20] and spin networks [21] has been
proposed as a way to establish short-range quantum
channels. The problem of what structures lead to high
fidelity state transfer has been of wide interest [21–23].
Here we show that it is possible to transfer, with low control
and high fidelity, a quantum state between two arbitrary
nonadjacent nodes of a random network (namely, an Erdös-
Renyi random graph). The Hamiltonian of a network of
coupled spins, with an XX type interaction, conserves the
number of excitations and so, in the single excitation
subspace, the Hamiltonian is that of a single particle
quantum walk on the same network. The graph \( G(n,p) \)
can be perceived as a communication network where each
node represents a party that transfers information to any of
the other nodes. We assume that each party has access to a
qubit and can control the local energy of the corresponding
node. In order to transfer a state from node \( i \) to \( j \),
with fidelity that tends to 1 in the asymptotic limit, the strategy
is the following: all qubits are initially in state \( |0\rangle \), which is an
eigenstate of the network; the sender (corresponding to
node \( i \)) performs a local operation on her qubit to prepare
\( |w\rangle = \alpha |0\rangle + \beta |1\rangle \). As long as \( p \geq \log^{3/2}(n)/n \), the approximate dynamics of a
quantum walk starting at \( |i\rangle \) is obtained by diagonalizing
the Hamiltonian

\[ H_{G(n,p)}' = -|i\rangle \langle i| - |j\rangle \langle j| - |s_w\rangle \langle s_w| - \gamma A_{G(n,p)}^i \]

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projected onto the approximately degenerate subspace spanned by \( \{ i \} , | s_{ij} \rangle , | j \} \), which is given by

\[
H'_{G(n,p)} = \begin{bmatrix}
-1 & -1/\sqrt{n} & 0 \\
-1/\sqrt{n} & -1 & -1/\sqrt{n} \\
0 & -1/\sqrt{n} & -1
\end{bmatrix},
\] (6)

with \( | s_{ij} \rangle = \sum_{k \neq i,j} | k \rangle / \sqrt{n-2} \) and \( | s_{ij} \rangle \approx | s_i \rangle \approx | s_j \rangle \), where we assume that \( i \) and \( j \) are nonadjacent vertices. Thus, the dynamics is approximately the same as that of end-to-end state transfer in a chain with three spins, where perfect state transfer is possible [23] and the component of the wave function at the receiver is approximately \( | \langle j | U(t) | i \rangle |^2 = \sin^2(t/\sqrt{2n}) \). Hence, after time \( T = \pi/\sqrt{n}/2 \), the receiver gets \( | y \rangle \) with fidelity 1, in the limit \( n \to \infty \) (see Fig. 2 for an example with finite \( n \)). The receiver can preserve this state for future use by tuning the energy of node \( j \), locally, to a value that is off-resonant with the rest of the network [24]. We conclude that high fidelity quantum state transfer can be achieved in almost all networks.

Creating Bell pairs in a random network.— In quantum communication networks, entanglement is an useful resource that can be used for various tasks such as teleportation, superdense coding, cryptographic protocols, etc [25]. Here, we present a protocol to entangle arbitrary nodes in a random network based on the search Hamiltonian. Imagine that Charlie at node \( | w \rangle \) wants to entangle the qubits of Alice at node \( | a \rangle \) and of Bob at node \( | b \rangle \). We assume that none of the nodes \( | w \rangle , | a \rangle , \) and \( | b \rangle \) are adjacent to each other. As before, \( \gamma \) is chosen to be \( 1/(np) \). In this case, the protocol is as follows: (i) Alice, Bob, and Charlie tune their respective site energies to \(-1\), (ii) Charlie tunes his nearest neighbor couplings to \( \sqrt{2}/d_C \), where \( d_C \) is the degree of the node corresponding to Charlie, while the other couplings in the graph are \( \gamma = 1/(np) \). This ensures that the Hamiltonian, projected onto the approximately degenerate subspace spanned by \(| w \rangle \), \( | s_{wab} \rangle = \sum_{k \neq a,b,w} | k \rangle / \sqrt{n-2} \) and \( | s_{ab} \rangle = (| a \rangle + | b \rangle )/\sqrt{2} \), is equal to

\[
H'_{G(n,p)} = \begin{bmatrix}
-1 & -\sqrt{2/n} & 0 \\
-\sqrt{2/n} & -1 & -\sqrt{2/n} \\
0 & -\sqrt{2/n} & -1
\end{bmatrix},
\] (7)

in the asymptotic limit [26]. Thus, after time \( T = \pi/\sqrt{n}/2 \), Alice and Bob share the state \( | s_{ab} \rangle = (| a \rangle + | b \rangle )/\sqrt{2} \), which is a Bell state. Subsequently, other Bell states may be obtained by local operations. Furthermore, Alice and Bob can preserve their Bell state by tuning the local energies of their qubits to a value that is off-resonant with the other eigenvalues of the network.

Discussion.— We have shown that searching for a marked node in a graph using continuous-time quantum walks works optimally for almost all graphs. This means that, in terms of the structures on which it performs optimally, this approach to quantum spatial search is much more general than what has been shown before. Our result was obtained by proving that the algorithm is almost surely optimal for Erdös-Rényi random graphs \( G(n,p) \), as long as \( p \geq \log^{3/2}(n)/n \).

As pointed out in Ref. [1], the analog version of Grover’s algorithm of Ref. [10] can be seen as a quantum walk on the complete graph. Furthermore, the Erdös-Rényi random graph \( G(n,p) \) can be obtained from the complete graph by randomly deleting edges with probability \( 1-p \). Thus, our result can also be interpreted as showing an inherent robustness of the analog version of Grover’s algorithm to edge loss. This implies that there is a large family of random Hamiltonians that can be employed to achieve optimal quantum search. Hence, our work paves the way to understanding how this randomness would translate to the circuit model of quantum search and whether this implies an inherent robustness of the (standard) Grover’s algorithm.

Finally, we have shown that one can adapt the spatial search algorithm to design protocols for quantum state transfer and for entanglement generation between arbitrary nodes of a random network of interacting qubits. Our results show that quantum information tasks typically designed for structured systems retain performance in very disordered structures. These results could lead to further investigation on what kind of random structures appear naturally in physical systems (for example, those appearing in Refs. [27,28]) and whether they would offer a sufficient spectral gap to perform efficient and robust quantum information tasks. It would also be interesting to explore whether nontrivial quantum information tasks can be performed on other models of random networks such as scale-free networks [29].

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[14] Normalized algebraic connectivity is defined as the second largest eigenvalue of the symmetric normalized Laplacian defined as $L' = D^{-1/2}LD^{-1/2}$, where $L$ is the Laplacian of the graph, with $D$ being a diagonal matrix where the $i$th diagonal entry is the degree of vertex $i$. In such a case we can define $H_1 = I - L'$.
[15] One of them is almost regular with $n - 2$ vertices having degree $n/2$, while the other two having degree $n/2 + 1$.
[24] The error in this analysis is in going up to only first order in degenerate perturbation theory.
[26] The state $|s_{ab}\rangle = (|a\rangle - |b\rangle)/\sqrt{2}$ is also degenerate with these states since $|s_{ab}\rangle H |s_{ab}\rangle \approx -1$. However, this state is decoupled from the dynamics because $|s_{\bar{a}\bar{b}}\rangle H |s_{\bar{a}\bar{b}}\rangle \approx -1$.