Quantum Searches on Highly Symmetric Graphs

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We study scattering quantum walks on highly symmetric graphs and use the walks to solve search problems on these graphs. The particle making the walk resides on the edges of the graph, and at each time step scatters at the vertices. All of the vertices have the same scattering properties except for a subset of special vertices. The object of the search is to find a special vertex. We consider, in particular, the complete graph and a complete bipartite graph. In both cases, the dimension d of the space in which the time evolution of the walk takes place is small (between $d = 3$ and $d = 6$), so the walks can be completely analyzed by the means of an analytical approach. Such dimensional reduction is due to the fact that these graphs have large automorphism groups. We find quantum speedups in all cases considered, approaching the Grover limit.

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I. INTRODUCTION

The theory of quantum walks describes quantum versions of classical random walks. In these walks a quantum particle “walking” on a line, or more generally a graph, has different amplitudes to go in different directions rather than different probabilities, which is the case for a classical walk. The time in these walks can either be in discrete steps [1]–[3] or continuous [4]. Both types of walks have proven to be fruitful sources of quantum algorithms [5]–[8]. A summary of both the properties of quantum walks and their algorithmic applications can be found in two recent reviews [9, 10].

Quantum walks have been used to investigate searches on a number of different graphs. In these searches, one of the vertices is distinguished, and the object is to find that vertex. The graphs considered so far are grids and hypercubes of different dimensions [11]–[13].

In this paper we will compare classical and quantum-walk searches on highly symmetric graphs. These graphs have large automorphism groups. In particular, we shall consider complete graphs (graphs in which there is an edge between any two vertices) and bipartite graphs in which each vertex in one of the two sets of vertices is connected to all of the vertices in the other set, but vertices within the sets are not connected to each other. We shall make use of the scattering quantum walk [14]. This is a discrete-time quantum walk in which the particle sits on the edges rather than the vertices of the graph, and at each step is scattered at the vertices. In some sense, scattering quantum walks are generalized coined quantum walks suitable for application on general graph structures. A natural example of such a walk is a photon that scatters on a set of beam splitters (vertices). We note that a quantum-walk search on a complete graph has been considered in [13] for the case of a continuous-time walk.

The proposed task may be described as follows: we are given a graph consisting of vertices and edges, and among the vertices, some are special. We want to find methods for finding a special vertex by the means of a quantum walk or a classical search, and then compare them. What we find is that because the graphs have large automorphism groups, a quantum walk starting in an equal superposition of all of the edge states stays within a subspace of small and constant dimension. The situation is analogous to that in the Grover search algorithm [15] in which the search takes place in a two-dimensional subspace. The result is that it is quite simple to find the behavior of the quantum search and compare it to the classical one. In addition, because the search becomes simple to analyze, we can study a whole class of special vertices. We find that some types are much better at producing quantum speedups than are others.

For a complete graph, we find that for the optimal choice of special vertex, the walk will locate it in $\mathcal{O}(\sqrt{N})$ steps, where N is the number of vertices in the graph. For the bipartite graph, with N_1 vertices in the first set an N_2 in the second, having a special vertex in set 1, but none in set 2, we find that the number of steps necessary to locate the special vertex is $\mathcal{O}(\sqrt{N_1})$; it does not depend on N_2. With one special vertex in each set, the number of steps does depend on both N_1 and N_2. However, if $N_2 \gg N_1$, then the number of steps in the walk will depend to good approximation only on N_1. On the other hand, in order to find the special vertex in the second set, the walk, of $\mathcal{O}(\sqrt{N_1})$ steps, will have to be repeated $\mathcal{O}(N_2/N_1)$ times for a total of $\mathcal{O}(N_2/\sqrt{N_1})$ steps.

The rest of the paper is organized as follows. First, in section II we discuss classical searches. In section III we will compare the performance of a classical search on a complete graph with one special vertex to that of the quantum search that utilizes scattering quantum walk. At the end of the section we provide the reader with a more general result for a complete graph with more than one special vertex. Section IV discusses the role of symmetry in the reduction of the dimensionality of the problem, and it is followed by an analysis of walks on bipartite graphs in section V.

II. CLASSICAL SEARCHES

If we consider a graph containing normal vertices, and special designated ones, which we are to find, then in the classical case, we may use several different approaches to accomplish this. We may perform classical searches either on vertices or on edges, where we pick edges and look at their ends in order to identify the special vertex. In the first case, the underlying graph structure is not taken into account. This would not be the case, if we would consider a random walk search — this, however, is not necessary, because the task is such that doing so does not bring any advantage. If the search is performed on edges, the underlying graph structure influences the choices we may make in the search for special vertex. As we will later see, this type of search is a classical reduction of the quantum walks that we study.

For both choices of the elements being searched, we may consider either a classical search without memory (blind search), where an element that has been chosen before can be chosen again, that is, we do not keep the track of elements which have already been examined, or we may consider a search having memory, in which every chosen element is noted and will not be chosen again. When searching directly on vertices, as we will see, these two procedures have essentially the same effectiveness (they differ only by a numerical factor), although search with memory is faster.

When comparing classical searches and quantum ones we need to carefully analyze the results. On one hand, we find, that the classical counterpart of the quantum walk we present is, as noted before, a *blind search*, which is never as fast as the quantum search. On the other hand, we may find in the classical case a faster search for special type of element. Comparing the effectiveness of such an algorithm and quantum walk search is possible, but has to be analyzed carefully due to the qualitative differences in resources both approaches use. We will not, however, address this matter in this paper. The comparison of both approaches will be based more on an analogy with the Grover speedup [15], while the issue of direct comparison based on (approximate) equivalence with Grover search will be addressed elsewhere [16].

A. Blind searches

Classical *blind searches* are searches where previously chosen elements are not noted, so that they may be picked again. This means that the probability P of choosing a special element remains the same after every unsuccessful step of the search. The probability of finding a special, or marked, element after k steps hence is

$$P_k = (1-P)^{k-1}P,$$

which is the probability of not finding the element in $k-1$ steps and finding it on the k-th step. The average number of steps we need to take in order to find a marked element is expressed via the sum

$$\bar{n} = \sum_{k=1}^{\infty} P_k k. \tag{2.1}$$

In the case of a blind search on vertices we have $P = v/N$ (v is the number of special vertices and N the total number of vertices in the graph) so that

$$\bar{n} = \frac{1}{P} = \frac{N}{v}. \tag{2.2}$$

If we are choosing edges instead of vertices, the situation gets more complicated. In such case, we not only choose an edge, but we must check its endpoints to see if one of them is a special vertex. Each of these operations is counted as one step. If the edge is not connected to a special vertex, then it contributes with three steps, one to pick it, and one step each to check the ends. An edge connected to two special vertices contributes with 2 steps, one to pick the edge and one to check one of the vertices (after we find a special vertex, we stop). If the edge is connected to one marked vertex, it contributes on average $1 + (1/2) + (1/2)2$ steps — one to choose it, and with probability 1/2 we pick the marked vertex first, and with probability 1/2 we pick it second. Therefore, in this case, if p_0 is the probability of choosing an edge with no special vertices, p_1 is the probability of choosing an edge with one special vertex, and p_2 is the probability of picking one with two, then

$$\bar{n} = \sum_{k=1}^{\infty} p_0^{k-1} \left\{ \left[3(k-1) + \frac{5}{2} \right] p_1 + [3(k-1)+2] p_2 \right\}. \tag{2.3}$$

B. Classical searches with memory

Now suppose that we note previously chosen elements, and do not choose them again in subsequent steps during the search. The probabilities P_k of finding a marked element now change for each new element chosen. In the case of a search on vertices we have

$$\begin{aligned} P_k &= \left[\frac{N-v}{N} \cdot \frac{N-v-1}{N-1} \cdots \right. \\ &\quad \left. \cdots \frac{N-v-k+2}{N-k+2} \right] \cdot \frac{v}{N-k+1} \\ &= \frac{(N-v)!v}{N!} \cdot \frac{(N-k)!}{(N-v-k+1)!}. \end{aligned}$$

This is a product of $(k-1)$ probabilities of not finding a special vertex on successive searches, where after each unsuccessful search we remove chosen normal vertex. In this case, the average number of steps taken in order to find a marked vertex is

$$\bar{n} = \sum_{k=1}^{N-v+1} P_k k. \tag{2.4}$$

After some evaluation this yields

$$\bar{n} = \frac{N+1}{v+1} \sim \frac{N}{v}. \tag{2.5}$$

We could also consider a search with memory on edges, but the evaluation of the average number of steps to find a marked element is somewhat involved. Since in this paper we will not need this kind of a search, we will not consider it further.

III. SEARCH ON A COMPLETE GRAPH

Let us now consider a complete graph with N vertices (see Fig. 1). Each vertex of this graph is connected to all of the other vertices by an edge, so the graph has $N(N-1)/2$ edges. Suppose that one vertex is special, which we can, without a loss of generality, take to be vertex 1, and that we would like to find it, under assumption that this special vertex has distinguishable properties from those of normal vertices, e.g. it may have different scattering properties as in Eq. (3.4) for special and in Eq. (3.2) for normal vertices. We shall now compare classical and quantum searches.

A. Classical case

Consider first a blind search on vertices where one does not need to take the internal structure of the graph into account. As we have seen in Eq. (2.2), the average number of steps that are needed to find the special vertex is N, since $v = 1$ in this case. For a blind search on edges, the resulting average number of steps, according to Eq. (2.3) is

$$\bar{n} = 3\left(\frac{N}{2} - 1\right) + \frac{5}{2}. \tag{3.1}$$

In this case, the number of steps again scales linearly with the number of vertices. Finally, the last considered classical search is a search on vertices with memory — we will make use of the results from section II B. Again the structure of the graph does not play role, and the average number of steps needed to find the special vertex is, as seen from Eq. (2.5), $(N+1)/2$ since again $v = 1$.

B. Quantum case

In order to describe our quantum walk, we need to define a Hilbert space and a unitary operator that advances the walk one step. The Hilbert space is spanned

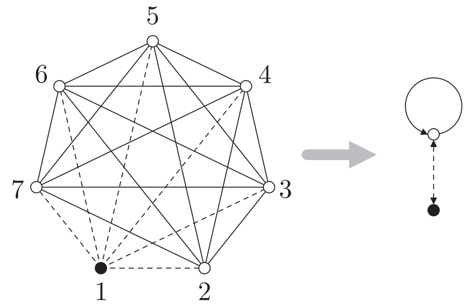

FIG. 1: A complete graph with $N = 7$ vertices out of which one is special (black one). The solution of the search in the quantum case leads to a reduction of dimensionality of the problem to 3 — there are three invariant subspaces under the action of $\hat{U}$. This is shown on the right-hand side of the picture: the superposition of edge states not connected to the special vertex create one such subspace and the superposition of edge states connected to the special vertex create another two such subspaces (one for each direction of particle — dashed double arrow).

by the edge states. There are two orthogonal states corresponding to each edge, one for each direction. That is, if an edge connects vertices j and k, the state $|j,k\rangle$ corresponds to the particle being on the edge between vertices j and k and going from j to k, while the state $|k,j\rangle$ corresponds to the particle being on the same edge, but going from k to j. Therefore, the dimension of the Hilbert space is $N(N-1)$, twice the number of edges.

Corresponding to each vertex there is a local unitary operator that relates the states coming into that vertex at one time step to the states going out of the vertex at the next time step, representing the scattering properties of the vertex/beam-splitter. The combined action of these local unitaries makes up the action of the overall unitary operator that advances the walk one time step. Without loss of generality, we can take the special vertex to be the vertex 1. For the vertices, $k \neq 1$ we have that

$$\hat{U}|j,k\rangle = -r|k,j\rangle + t \sum_{\substack{a=1 \\ a\neq j,k}}^{N} |k,a\rangle, \tag{3.2}$$

where $\hat{U}$ is the operator that advances the walk one time step, and the transmission and reflection coefficients are

$$t = \frac{2}{N-1} \qquad r = \frac{N-3}{N-1}. \tag{3.3}$$

Such a unitary corresponds to the usual choice of a Grover coin in coined quantum walks [17]. Note that $r + t = 1$ and, as unitarity requires,

$$r^2 + (N-2)t^2 = 1.$$

The operator $\hat{U}$ reflects the symmetry of the graph, i.e. each edge coming into a vertex is treated in the same way.

At vertex 1 we have

$$\hat{U}|j,1\rangle = \mathrm{e}^{\mathrm{i}\phi}|1,j\rangle, \tag{3.4}$$

where we shall examine the effect of different choices of *phase shift* ϕ later. Needless to say, this vertex also respects the symmetry of the graph.

Let us now consider the three orthonormal vectors

$$\begin{aligned} |w_1\rangle &= \frac{1}{\sqrt{N-1}}\sum_{j=2}^{N}|j,1\rangle; \\ |w_2\rangle &= \frac{1}{\sqrt{N-1}}\sum_{j=2}^{N}|1,j\rangle; \\ |w_3\rangle &= \frac{1}{\sqrt{(N-1)(N-2)}}\sum_{j=2}^{N}\sum_{\substack{k=2\\k\neq j}}^{N}|j,k\rangle. \end{aligned}$$

These vectors are, respectively, superpositions of edge states going into the vertex 1, edge states going out of the vertex 1, and edge states that do not start or finish on the vertex 1. The subspace they span, which we shall call S, is invariant under the action of $\hat{U}$. This can be seen from the action of unitary evolution operator $\hat{U}$:

$$\begin{aligned} \hat{U}|w_1\rangle &= \mathrm{e}^{\mathrm{i}\phi}|w_2\rangle; \\ \hat{U}|w_2\rangle &= -r|w_1\rangle + t\sqrt{N-2}|w_3\rangle; \\ \hat{U}|w_3\rangle &= t\sqrt{N-2}|w_1\rangle + r|w_3\rangle. \end{aligned}$$

This means that $\hat{U}$ restricted to S, which we shall call $\hat{U}_S$, is just a 3×3 matrix, which, in the basis $\{|w_j\rangle \mid j = 1,2,3\}$, is given by

$$\hat{U}_S = \begin{pmatrix} 0 & -r & t\sqrt{N-2} \\ \mathrm{e}^{\mathrm{i}\phi} & 0 & 0 \\ 0 & t\sqrt{N-2} & r \end{pmatrix}. \tag{3.5}$$

We also note that the vector that is an equal superposition of all edge states,

$$|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{N(N-1)}}\sum_{j=1}^{N}\sum_{\substack{k=1\\k\neq j}}^{N}|j,k\rangle, \tag{3.6}$$

which is the state in which we start the walk, is given by

$$|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{N}}(|w_1\rangle + |w_2\rangle) + \sqrt{\frac{N-2}{N}}|w_3\rangle,$$

so that it too is in S. Therefore, our entire walk starting in $|\psi_{\text{initial}}\rangle$, takes place in the subspace S, and what first seemed to be an $N(N-1)$-dimensional problem has been reduced to a three-dimensional one. As we shall see, this is a consequence of the symmetry of the graph and the fact that the unitary time-step operator does not break this symmetry.

Our next task is to find the eigenstates and eigenvalues of $\hat{U}_S$ in order to be able to describe the overall evolution of $|\psi_{\text{initial}}\rangle$ according to Eq. (3.7). We shall consider two cases, $\phi = 0$ and $\phi = \pi$, and we shall find that properties of $\hat{U}_S$ in these two cases are very different. In the case $\phi = 0$, it suffices to note that one of the eigenvalues of $\hat{U}_S$ is 1, and the eigenvector corresponding to this eigenvalue is just $|\psi_{\text{initial}}\rangle$. That means that successive applications of $\hat{U}_S$ do not change the state, and the walk does nothing; the state of the walk after n steps is the same as the initial state of the walk. In this case the walk is useless in finding the special vertex since it reduces to a classical blind search (the efficiency of the algorithm shall be considered more closely in next subsection). The situation for $\phi = \pi$ is very different.

For the case $\phi = \pi$, $\hat{U}_S$ has the eigenvalue $\lambda = -1$ with corresponding eigenvector

$$|\tilde{u}_0\rangle = \sqrt{\frac{N-2}{2N-3}}\begin{pmatrix} 1 \\ 1 \\ \frac{-1}{\sqrt{N-2}} \end{pmatrix},$$

and the eigenvlaues

$$\lambda = \mathrm{e}^{\pm\mathrm{i}\theta} = \frac{1}{N-1}[(N-2) \pm \mathrm{i}\sqrt{2N-3}],$$

with corresponding eigenvectors

$$|\tilde{u}_\pm\rangle = \sqrt{\frac{N-1}{2(2N-3)}}\begin{pmatrix} -\mathrm{e}^{\pm\mathrm{i}\theta} \\ 1 \\ \frac{\sqrt{N-2}}{N-1}[1 \mp \mathrm{i}\sqrt{2N-3}] \end{pmatrix},$$

where $\tan\theta = \sqrt{2N-3}/(N-2)$. We can now find the state of the walk after n steps from the equation

$$\begin{aligned} \hat{U}^n|\psi_{\text{initial}}\rangle &= (-1)^n|\tilde{u}_0\rangle\langle\tilde{u}_0|\psi_{\text{initial}}\rangle \\ &\quad + \mathrm{e}^{in\theta}|u_+\rangle\langle u_+|\psi_{\text{initial}}\rangle \\ &\quad + \mathrm{e}^{-in\theta}|\tilde{u}_-\rangle\langle\tilde{u}_-|\psi_{\text{initial}}\rangle. \end{aligned} \tag{3.7}$$

Setting $\zeta = 1 + \mathrm{i}\sqrt{2N-3}$, this becomes

$$\begin{aligned} \hat{U}^n|\psi_{\text{initial}}\rangle &= (-1)^n\frac{N-2}{(2N-3)\sqrt{N}}\begin{pmatrix} 1 \\ 1 \\ \frac{-1}{\sqrt{N-2}} \end{pmatrix} \\ &\quad + \frac{N-1}{2(2N-3)\sqrt{N}}\begin{pmatrix} \zeta^*\mathrm{e}^{in\theta} + \zeta\mathrm{e}^{-in\theta} \\ \zeta\mathrm{e}^{in\theta} + \zeta^*\mathrm{e}^{-in\theta} \\ 4\sqrt{N-2}\cos(n\theta) \end{pmatrix}. \end{aligned}$$

Note that the first term is of order $1/\sqrt{N}$ and the second is of order 1, so for large N we need only consider the second term. We see that initially it is the $|w_3\rangle$ component that is largest, indicating that it is most likely that the particle will be found on an edge not connected to the special vertex. When $n\theta \cong \pi/2$, however, it is the $|w_1\rangle$ and $|w_2\rangle$ components that are of the order 1, while the $|w_3\rangle$ is of the order $1/\sqrt{N}$. This means that the particle is overwhelmingly likely to be located on an edge that is connected to the special vertex. Therefore, at this time we simply measure the particle in order to find which

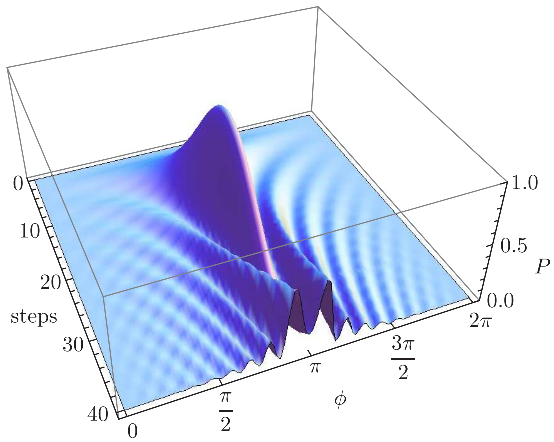

FIG. 2: (Color on-line) Numerical results for the complete graph with $N = 256$ vertices showing the evolution of a probability P for particle being on edge connected to the special vertex and its dependence on ϕ. Moving away from $\phi = \pi$ causes time oscillations of the probability to decrease in the amplitude and increase in the frequency, while approaching the value 0. In this sense $\phi = \pi$ is optimal for the quantum search.

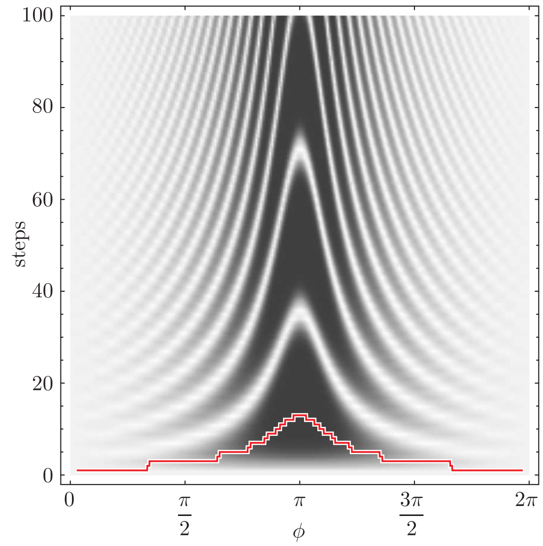

FIG. 3: (Color on-line) Density plot of the probability P, taken for $N = 256$, shows the convergence of the side-ridges to the maximum (dark gray) for $\phi = \pi$ with the probability $P = 1$. White areas correspond to minimal probability of finding particle on edge connected to the special vertex. The thick red line represents optimal number of steps that are to be taken before the measurement so that the algorithm for the special vertex search would require minimal average number of steps.

edge it is located on, and then check the vertices at the ends of this edge. One of these vertices is very likely to be the special one. Noting that $\theta \cong \sqrt{2/N}$, we see that we can find the special vertex by running the walk for $\mathcal{O}(\sqrt{N})$ steps. This represents a quadratic speedup over a classical search, e.g. a blind search on edges which is, as we will soon see, the closest classical counterpart for the quantum search.

C. Role of the phase-shift

As we have seen previously, the differences between the phase-shift being 0 and π are substantial. To see how this change occurs we will present some numerical results for $0 \leq \phi < 2\pi$. The behavior of the walk is depicted in Fig. 2, where we see, that the further we are from $\phi = \pi$, the smaller is the probability P of finding particle on an edge that is connected to the special vertex.

Another thing we can observe from Fig. 2 is the symmetry in ϕ — the situation looks much the same for ϕ going from 2π to π as for ϕ going from 0 to π. This property can be shown in the following way. If we apply the substitution $\phi \to 2\pi - \phi$ in the unitary $\hat{U}_S$ from Eq. (3.5) we obtain change of $\hat{U}_S$ to $\hat{U}_S^*$. This result together with the fact, that the initial state has real components, yields

$$\left(\hat{U}_S^*\right)^n |\psi_{\text{initial}}\rangle = \left(\hat{U}_S^*\right)^n |\psi_{\text{initial}}^*\rangle = \left(\hat{U}_S^n |\psi_{\text{initial}}\rangle\right)^*.$$

So the resulting components are now the complex conjugates of the original; however, the probabilities remain the same.

The value $\phi = \pi$ is special, because for any other ϕ the probability P never reaches one. This can be seen both in Fig. 2 and Fig. 3. The significance of $\phi = \pi$ leads to the following question. Suppose we are given a complete graph having one special vertex with an arbitrary but known phase-shift. Our task is to find the special vertex. In order to find it efficiently, we need to wait for the optimal number of steps before performing the measurement. If we were given only one chance to measure, we would have to wait until the probability of finding particle on the edge connected to the special vertex reaches its maximum. However, if we are able to repeat the experiment an arbitrary number of times, we may, after an unsuccessful search, do the experiment again. In that case, the optimal number of steps before measuring would be different — it would be the number of steps, for which the *average number of steps* is minimal. Let $P_\phi(m)$ be the probability of finding the particle on an edge connected to the special vertex after one repeat of the experiment assuming that m steps are taken before measurement, and the phase-shift is ϕ. Then the average number of steps $\bar{n}_{\phi,m}$ to be taken when measuring after m steps on a graph with phase-shift ϕ is given by

$$\bar{n}_{\phi,m} = \sum_{k=1}^{\infty} P_{\phi,m}(k) k m,$$

where

$$P_{\phi,m}(k) = [1 - P_\phi(m)]^{k-1} P_\phi(m)$$

is the probability of finding the particle on an edge connected to the special vertex after k repeats of the ex-

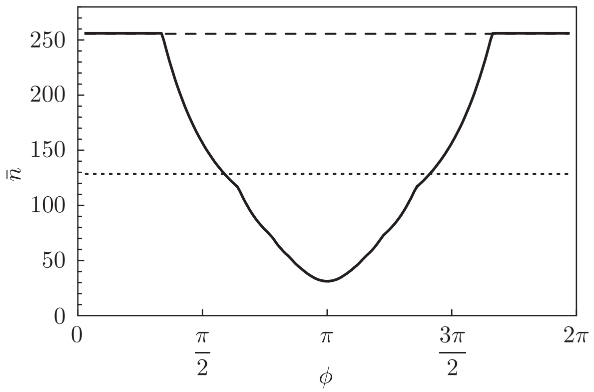

FIG. 4: Efficiency of algorithms — classical blind search (dashed), classical search with memory (dotted) and quantum search (thick solid). The graph was taken for $N = 256$.

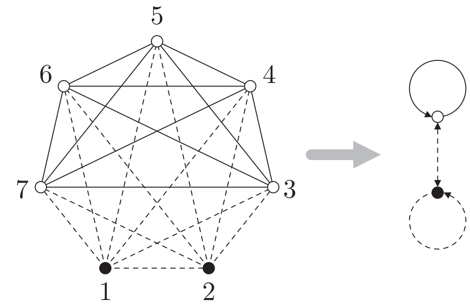

FIG. 5: Example of a complete graph with $N = 7$ vertices out of which $v = 2$ are special (black ones). Solution for scattering quantum walk on such graphs leads to a reduction in dimensionality of the problem to four dimensions, which is indicated on the right-hand side of the figure.

periment (and no sooner). After a short evaluation we find

$$\bar{n}_{\phi,m} = \frac{m}{P_\phi(m)}.$$

The optimal number of steps, $m_{\rm opt}$, in each experiment is given by the value of m that minimizes $n_{\phi,m}$. We will denote the average number of steps to be taken in optimal case as $\bar{n}(\phi) = \bar{n}_{\phi,m_{\rm opt}}$.

From the preceding, it is clear, that for $\phi = \pi$ the quantum approach is faster than the classical, it has a quadratic speedup, even in the non-optimal search via maximum probability method (see Fig. 4). However, for the case of $\phi \sim 0$ we see that the optimal number of steps is 0 — we do not evolve the system, we just measure the initial state — and the average number of steps reaches a value close to N. This is the same situation we would have if we performed a classical blind search where we randomly pick vertices at each step without remembering the past choices.

So the quantum search transforms into the classical blind search on edges for $\phi \sim 0$ (2π), which can be, in this sense, considered as its classical counterpart. If ϕ approaches π, the quantum search becomes not only faster but also more efficient then the classical one.

D. Complete graph with more than one special vertex

We may also consider a graph that has more than one special vertex (as for example in Fig. 5). In this case the solution is similar to the solution for one special vertex.

First suppose, without a loss of generality, that vertices $k = 1, 2, \dots v$ are special with the evolution operator for these vertices being (where $j \neq k$)

$$U|j,k\rangle = \mathrm{e}^{\mathrm{i}\phi}|k,j\rangle.$$

Vertices $v+1, v+2, \dots, N$ are *normal* and the evolution operator from Eq. (3.2) remains the same. The transmission and reflection coefficients t and r from Eq. (3.3) are also the same.

The dimensionality of the problem in this case, however, is not reduced to three as in the previous case. Due to the fact, that there are also edge states for which there is a special vertex on both ends of the edge, we have to add another orthogonal state — $|w_4\rangle$ — and rescale the amplitudes so that:

$$\begin{aligned}
|w_1\rangle &= \frac{1}{\sqrt{v(N-v)}} \sum_{a=v+1}^{N} \sum_{b=1}^{v} |a,b\rangle; \\
|w_2\rangle &= \frac{1}{\sqrt{v(N-v)}} \sum_{a=1}^{v} \sum_{b=v+1}^{N} |a,b\rangle; \\
|w_3\rangle &= \frac{1}{\sqrt{(N-v)(N-v-1)}} \sum_{a=v+1}^{N} \sum_{\substack{b=v+1 \\ b\neq l}}^{N} |a,b\rangle; \\
|w_4\rangle &= \frac{1}{\sqrt{v(v-1)}} \sum_{a=1}^{v} \sum_{\substack{b=1 \\ m\neq l}}^{v} |a,b\rangle.
\end{aligned}$$

Unitary evolution for these states changes accordingly:

$$\begin{aligned}
\hat{U}|w_1\rangle &= \mathrm{e}^{\mathrm{i}\phi}|w_2\rangle; \\
\hat{U}|w_2\rangle &= [-r + t(v-1)]|w_1\rangle + t\sqrt{v(N-v-1)}|w_3\rangle; \\
\hat{U}|w_3\rangle &= t\sqrt{v(N-v-1)}|w_1\rangle + [r - t(v-1)]|w_3\rangle,
\end{aligned}$$

with the additional equation for $|w_4\rangle$

$$\hat{U}|w_4\rangle = \mathrm{e}^{\mathrm{i}\phi}|w_4\rangle.$$

This leads to a 4×4 matrix $\hat{U}_S$ restricted to S — the subspace spanned by the vectors $|w_k\rangle, k = 1, 2, 3, 4$:

$$\hat{U}_S = \begin{pmatrix} 0 & q & s & 0 \\ \mathrm{e}^{\mathrm{i}\phi} & 0 & 0 & 0 \\ 0 & s & -q & 0 \\ 0 & 0 & 0 & \mathrm{e}^{\mathrm{i}\phi} \end{pmatrix},$$

where

$$
\begin{aligned}
q &= -r + t(v-1) = -1 + \frac{2v}{N-1}; \\
s &= \sqrt{1-q^2} = t\sqrt{v(N-u-1)}; \\
q^2 + s^2 &= 1.
\end{aligned}
$$

Note that the subspace spanned by the vectors $|w_k\rangle, k = 1,2,3$ is decoupled from the subspace spanned by the vector $|w_4\rangle$. Note that for $v \ll N$ we have $q = -1 + x$ with $x \sim 1/N$ and $s \sim 1/\sqrt{N}$. The initial state from Eq. (3.6) can now be written in form

$$
\begin{aligned}
|\psi_{\rm initial}\rangle &= \sqrt{\frac{(N-v)(N+v-1)}{N(N-1)}}|\tilde{u}_0\rangle \\
&\quad + \sqrt{\frac{v(v-1)}{N(N-1)}}|\tilde{u}_0'\rangle,
\end{aligned}
$$

where $|\tilde{u}_0\rangle$ and $|\tilde{u}_0'\rangle$ are orthogonal eigenstates of $\hat{U}_S$ for $\phi = 0$ with eigenvalue 1:

$$
\begin{aligned}
|\tilde{u}_0'\rangle &= (0,0,0,1)^{\rm T}; \\
|\tilde{u}_0\rangle &= \sqrt{\frac{1+q}{3+q}} \begin{pmatrix} 1 \\ 1 \\ \sqrt{\frac{1-q}{1+q}} \\ 0 \end{pmatrix}.
\end{aligned}
$$

As in the previous case, for $\phi = 0$ we may observe just a trivial time evolution giving no advantage over classical searches.

The value of $\phi = \pi$ is again special. The state of the walk after n steps, derived in similar manner as in the case for $v = 1$, is

$$
\begin{aligned}
\hat{U}^n|\psi_{\rm initial}\rangle &= (-1)^n \frac{v(v-1)}{N(N-1)} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} + \sqrt{\frac{v(N-v)(N-1)}{4(2N-v-2)^2 N}} \begin{pmatrix} \zeta^* {\rm e}^{in\theta} + \zeta {\rm e}^{-in\theta} \\ \zeta {\rm e}^{in\theta} + \zeta^* {\rm e}^{-in\theta} \\ 4\sqrt{(N-v-1)/v}\cos n\theta \\ 0 \end{pmatrix} \\
&\quad + (-1)^n \frac{N-v-1}{2N-v-2} \sqrt{\frac{v(N-v)}{N(N-1)}} \begin{pmatrix} 1 \\ 1 \\ -\sqrt{\frac{v}{N-v-1}} \\ 0 \end{pmatrix},
\end{aligned}
$$

where

$$
\begin{aligned}
\zeta &= 1 + {\rm i}\sqrt{\frac{v(N-v)}{N(N-1)}}, \\
\tan\theta &= \frac{\sqrt{v(2N-v-2)}}{N-v-1}.
\end{aligned}
$$

We see analogous behavior as for $v = 1$ — the probability amplitudes for edge states not connected to special vertices decay to zero when $\theta n = \pi/2$, especially for large N, when the third term approaches zero. This implies that the number of steps needed to find one of the special vertices is of order $\mathcal{O}(\sqrt{N/v})$ for $N \gg v \geq 1$ which is again a quadratic speedup over the classical algorithm that needs $\mathcal{O}(N/v)$ steps, as seen from Eq. (2.2), for example.

IV. SYMMETRY CONSIDERATIONS

One obvious question that occurs after the previous analysis is why a quantum walk on a graph whose Hilbert space has $N(N-1)$ dimensions takes place in a subspace of only three or four dimensions. Here we shall try to gain some insight into the answer by studying the role played by the symmetry properties of the graph.

Suppose we have again a graph with one special vertex, and let $\mathcal{A}$ be the group of automorphisms of the graph that leave the special vertex fixed. If V is the set of vertices of a graph, G, then an automorphism a of G is a mapping, $a: V \rightarrow V$ such that for any vertices $v_1, v_2 \in V$, there is an edge connecting $a(v_1)$ and $a(v_2)$ if and only if there is an edge connecting v_1 and v_2. The Hilbert space of the graph, $\mathcal{H}_G$, is just the span of the basis states corresponding to the particle being on an edge and going from one vertex to another, i.e. if there is an edge between vertices v_1 and v_2, then the basis states corresponding to this edge are $|v_1, v_2\rangle$ (going from v_1 to v_2) and $|v_2, v_1\rangle$ (going from $v_2$to v_1). We shall refer to this basis as the canonical basis for $\mathcal{H}_G$. Each automorphism, a, induces a unitary mapping on the Hilbert space of the graph, $\hat{U}_a$, such that $\hat{U}_a|v_1, v_2\rangle = |a(v_1), a(v_2)\rangle$. Suppose now that $\mathcal{H}_G$ can be decomposed into subspaces,

$$
\mathcal{H}_G = \bigoplus_{j=1}^{m} \mathcal{H}_j,
$$

where each $\mathcal{H}_j$ is the span of some subset, B_j of the canonical basis elements and is invariant under $\hat{U}_a$ for all $a \in \mathcal{A}$. We shall also assume that each $\mathcal{H}_j$ does not contain any smaller invariant subspaces.

Note that our example, the complete graph with one special vertex, has this structure. The automorphism group consists of all permutations of the vertices that leave vertex 1 fixed. The invariant subspaces are $\mathcal{H}_1 = \text{span}\{|j,1\rangle | j = 2, \ldots N\}$, $\mathcal{H}_2 = \text{span}\{|1,j\rangle | j = 2, \ldots N\}$, and $\mathcal{H}_3 = \text{span}\{|j,k\rangle | j,k = 2, \ldots N, k \neq j\}$.

Next, in each invariant subspace we can form a vector that is the sum of all of the canonical basis elements in the subspace,

$$|w_j\rangle = \frac{1}{\sqrt{d_j}} \sum_{\{v_1,v_2| \ |v_1,v_2\rangle \in B_j\}} |v_1, v_2\rangle, \qquad (4.1)$$

where d_j is the dimension of $\mathcal{H}_j$. This vector satisfies $\hat{U}_a|w_j\rangle = |w_j\rangle$ for all $a \in \mathcal{A}$, and it is the only vector in $\mathcal{H}_j$ that satisfies this condition. Define $S = \text{span}\{|w_j\rangle | j = 1, \ldots m\}$, and note that $S = \{|\psi\rangle \in \mathcal{H}_G \ |\hat{U}_a|\psi\rangle = |\psi\rangle \ \forall a \in \mathcal{A}\}$, and that the dimension of S is simply the number of invariant subspaces. Now suppose that $[\hat{U}, \hat{U}_a] = 0$ for all $a \in \mathcal{A}$. This implies that if $\hat{U}_a|\psi\rangle = |\psi\rangle$, then $\hat{U}_a\hat{U}|\psi\rangle = \hat{U}|\psi\rangle$, i.e. if $|\psi\rangle \in S$, then $\hat{U}|\psi\rangle \in S$. Therefore, the subspace S is closed under the action of the time-step operator $\hat{U}$, and if the initial state of the walk is in S, then we only need to consider states in S to describe the state of the walk at any time. If the automorphism group is large, then S can have a much smaller dimension than $\mathcal{H}_G$.

Now let us demonstrate that the unitary operator we are using to move the walk forward one step does, in fact, commute with all of the automorphisms of a graph that leave the special vertex fixed. If these operators commute when applied to all of the elements of the canonical basis, then they commute. Let $\Gamma(v)$ be the set of vertices in G that are connected to the vertex v, and, if $v' \in \Gamma(v)$ let $\Gamma(v; v') = \Gamma(v) - v'$. Then let us assume that if v_2 is not a special vertex (we shall treat this case shortly), then the operator $\hat{U}$ acts on states in the canonical basis as

$$\hat{U}|v_1, v_2\rangle = -r|v_2, v_1\rangle + t \sum_{v \in \Gamma(v_2; v_1)} |v_2, v\rangle, \qquad (4.2)$$

where the transmission and reflection amplitudes depend only on the number of elements in $\Gamma(v_2)$, which we denote by $|\Gamma(v_2)|$. Next, we have that

$$\hat{U}_a\hat{U}|v_1, v_2\rangle = -r|a(v_2), a(v_1)\rangle + t \sum_{v \in \Gamma(v_2; v_1)} |a(v_2), a(v)\rangle. \qquad (4.3)$$

We also have

$$\hat{U}\hat{U}_a|v_1, v_2\rangle = -r|a(v_2), a(v_1)\rangle + t \sum_{v \in \Gamma(a(v_2); a(v_1))} |a(v_2), v\rangle. \qquad (4.4)$$

First note that the reflection and transmission amplitudes in this equation are the same as those in the previous equation, because $|\Gamma(v_2; v_1)| = |\Gamma(a(v_2); a(v_1))|$. We also have that $\Gamma(a(v_2); a(v_1)) = \{a(v)| \ v \in \Gamma(v_2; v_1)\}$, so that the sums in the two equations are identical. Therefore, $U_a\hat{U}|v_1, v_2\rangle = \hat{U}\hat{U}_a|v_1, v_2\rangle$. If v_2 is a special vertex, then $\hat{U}|v_1, v_2\rangle = e^{i\phi}|v_2, v_1\rangle$, so that

$$\hat{U}_a\hat{U}|v_1, v_2\rangle = \hat{U}\hat{U}_a|v_1, v_2\rangle = e^{i\phi}|v_2, a(v_1)\rangle. \qquad (4.5)$$

Therefore, the operators $\hat{U}$ and $\hat{U}_a$ commute for all automorphisms of the graph, a, that leave the special vertex fixed.

For the complete graph considered in the previous section, we do have $[\hat{U}, \hat{U}_a] = 0$ and the vectors $|w_j\rangle$, $j = 1, 2, 3$, are just the vectors defined in Eq. (4.1) for the subspaces $\mathcal{H}_j$, $j = 1, 2, 3$. This, then, explains the reduction of the search on the complete graph from an $N(N-1)$ dimensional problem to a three-dimensional one.

These symmetry considerations also hold for graphs with an arbitrary number of special vertices. As we saw in the previous section, in the case of a complete graph increasing the number of special vertices increased the dimension of the problem from three to four.

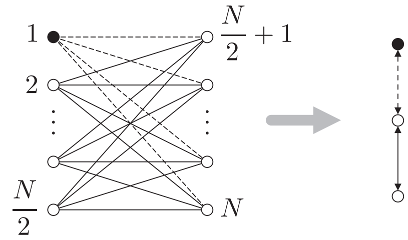

FIG. 6: A bipartite graph with $N/2$ vertices in both sets (N is even). Vertex 1 is special (black circle). This problem reduces to a four-dimensional problem depicted on the right in the same manner as before.

V. BIPARTITE GRAPH

Now let us have a look at a quantum search on a graph with a bit less symmetry than a complete graph. We shall consider a bipartite graph (see Fig. 6) with N vertices (N is even), in which vertices 1 through $N/2$ are in the first set (left in Fig. 6) and vertices $(N/2) + 1$ to N are in the second set (right in Fig. 6). There is an edge between each vertex in the first set and each vertex in the second set, but there are no edges connecting vertices within the same set. Therefore, the total number of edges is $(N/2)^2$ and the dimension of $\mathcal{H}_G$ is $N^2/2$.

As before, we will take vertex 1 to be our special vertex, and it behaves as before [see Eq. (3.4)]. The other vertices also behave as in the previous example, see Eq. (3.2), but in this case, since each vertex has $N/2$ edges connected to it, we have

$$t = \frac{4}{N} \qquad r = \frac{N-4}{N}.$$

In this case, the group of automorphisms, $\mathcal{A}$, of the graph consist of permutations of the vertices within the sets that leave vertex 1 fixed. There are four invariant subspaces. The first is the subspace consisting of all vectors entering vertex 1, and the vector

$$|w_1\rangle = \sqrt{\frac{2}{N}} \sum_{j=(N/2)+1}^{N} |j,1\rangle$$

is the vector in this space that is an eigenvector of $\hat{U}_a$, for all $a \in \mathcal{A}$, with eigenvalue one. The second invariant subspace consists of vectors leaving vertex 1, and the corresponding vector is

$$|w_2\rangle = \sqrt{\frac{2}{N}} \sum_{j=(N/2)+1}^{N} |1,j\rangle.$$

The third invariant subspace consists of all vectors leaving vertices 2 through $N/2$, with corresponding vector

$$|w_3\rangle = \frac{2}{\sqrt{N(N-2)}} \sum_{j=2}^{N/2} \sum_{k=(N/2)+1}^{N} |j,k\rangle,$$

and the fourth consists of all vectors entering vertices 2 through $N/2$, with corresponding vector

$$|w_4\rangle = \frac{2}{\sqrt{N(N-2)}} \sum_{j=2}^{N/2} \sum_{k=(N/2)+1}^{N} |k,j\rangle.$$

The subspace S, in which the walk takes place is simply the linear span of the orthonormal vectors $|w_1\rangle, \ldots, |w_4\rangle$. The time step operator, $\hat{U}$, has the action

$$\begin{aligned}
\hat{U}|w_1\rangle &= \mathrm{e}^{\mathrm{i}\phi}|w_2\rangle; \\
\hat{U}|w_2\rangle &= -r|w_1\rangle + t\sqrt{\frac{N-2}{2}}|w_4\rangle; \\
\hat{U}|w_3\rangle &= t\sqrt{\frac{N-2}{2}}|w_1\rangle + r|w_4\rangle; \\
\hat{U}|w_4\rangle &= |w_3\rangle,
\end{aligned}$$

which implies that the matrix of $\hat{U}$ restricted to S, $\hat{U}_S$, is, in the basis $\{|w_j\rangle \; |j = 1,2,3,4\}$,

$$\hat{U}_S = \begin{pmatrix} 0 & -r & t\sqrt{\frac{N-2}{2}} & 0 \\ \mathrm{e}^{\mathrm{i}\phi} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & t\sqrt{\frac{N-2}{2}} & r & 0 \end{pmatrix}.$$

As before, we shall examine the cases $\phi = 0$ and $\phi = \pi$.

In the case $\phi = 0$, the eigenvalues of $\hat{U}_S$ are $\pm 1, \pm\mathrm{i}$. The eigenvector corresponding to 1 is

$$|u_+\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 \\ 1 \\ \sqrt{\frac{N-2}{2}} \\ \sqrt{\frac{N-2}{2}} \end{pmatrix},$$

and the eigenvector corresponding to -1 is

$$|u_-\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 \\ -1 \\ -\sqrt{\frac{N-2}{2}} \\ \sqrt{\frac{N-2}{2}} \end{pmatrix}.$$

The obvious vectors in which to start the walk are the ones consisting of all edges entering the first set, which is just $(|u_+\rangle + |u_-\rangle)/\sqrt{2}$, the vector consisting of all edges leaving the first set, which is just $(|u_+\rangle - |u_-\rangle)/\sqrt{2}$, or some linear combination of them, possibly equal superposition of all edge states, which is $|u_+\rangle$. None of these starting vectors is useful in finding the special vertex. The state of the walk simply oscillates with a period of two steps. Therefore, we conclude that, as in the case of the complete graph, we cannot utilize such quantum walk to find the special vertex in the case $\phi = 0$.

Let us now look at the case $\phi = \pi$. The eigenvalues are given by the solutions to the equation

$$\lambda^2 = r \pm i(1-r^2)^{1/2}.$$

Defining $\tan\eta = \sqrt{1-r^2}/r$, so that $\cos\eta = r$ and $\sin\eta = \sqrt{1-r^2} = t\sqrt{(N-2)/N} = \mathcal{O}(1/\sqrt{N})$, we have that the eigenvalues and eigenvectors are: $\lambda = \mathrm{e}^{\mathrm{i}\eta/2}$ with the eigenvector

$$|u_1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\mathrm{e}^{-\mathrm{i}\eta/2} \\ \mathrm{i}\mathrm{e}^{-\mathrm{i}\eta/2} \\ \mathrm{i} \end{pmatrix},$$

$\lambda = -\mathrm{e}^{\mathrm{i}\eta/2}$ with the eigenvector

$$|u_2\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \mathrm{e}^{-\mathrm{i}\eta/2} \\ -\mathrm{i}\mathrm{e}^{-\mathrm{i}\eta/2} \\ \mathrm{i} \end{pmatrix},$$

$\lambda = \mathrm{e}^{-\mathrm{i}\eta/2}$ with the eigenvector

$$|u_3\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -\mathrm{e}^{\mathrm{i}\eta/2} \\ -\mathrm{i}\mathrm{e}^{\mathrm{i}\eta/2} \\ -\mathrm{i} \end{pmatrix},$$

$\lambda = -\mathrm{e}^{-\mathrm{i}\eta/2}$ with the eigenvector

$$|u_4\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ \mathrm{e}^{\mathrm{i}\eta/2} \\ \mathrm{i}\mathrm{e}^{\mathrm{i}\eta/2} \\ -\mathrm{i} \end{pmatrix}.$$

As an initial state, let us consider the state consisting of an equal superposition of all edge states (in fact any state in the subspace spanned by $|u_+\rangle$ and $|u_-\rangle$ would also work as is shown later in general case — see Sec. V A.), which is given by

$$|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{N}} \begin{pmatrix} 1 \\ 1 \\ \sqrt{\frac{N-2}{N}} \\ \sqrt{\frac{N-2}{N}} \end{pmatrix}.$$

The state of the walk after n steps is given by

$$\hat{U}^n |\psi_{\text{initial}}\rangle = \sum_{j=1}^{4} \lambda_j^n |u_j\rangle\langle u_j|\psi_{\text{initial}}\rangle.$$

We find that $|\langle u_j|\psi_{\text{initial}}\rangle|$ is of order one for $j = 1, 3$ and of order $1/\sqrt{N}$ for $j = 2, 4$. Keeping only the $j = 1, 3$ terms, while dropping additional terms that are of the order $1/\sqrt{N}$ and smaller, we find that

$$\hat{U}^n |\psi_{\text{initial}}\rangle = \frac{1}{2\sqrt{2}} \begin{pmatrix} \sin[(n+1)\eta/2] + \sin(n\eta/2) \\ -\sin(n\eta/2) - \sin[(n-1)\eta/2] \\ \cos(n\eta/2) + \cos[(n-1)\eta/2] \\ \cos[(n+1)\eta/2] + \cos(n\eta/2) \end{pmatrix}.$$

When $n\eta = \pi$ the last two components of the above vector are approximately zero, while the first two are approximately $1/\sqrt{2}$. This corresponds to the particle being on edges entering and leaving the special vertex. As before, after $n \cong \pi/\eta = \mathcal{O}(\sqrt{N})$ steps, we measure in the canonical basis to find the edge on which the particle is located, and then check the vertices to see if one of them is the special one. With overwhelming probability, it will be, and we have found the special vertex in $\mathcal{O}(\sqrt{N})$ steps. We have again achieved quadratic speedup over classical counterpart — blind search on edges where we would have to make $\mathcal{O}(N)$ steps on average to find the special vertex.

A. General bipartite graph with special vertices in only one set

Previous results can as well be generalized to a bipartite graph that has v special vertices (labeled from 1 to v) together with m normal vertices (labeled from $v+1$ to $v+m$) in first set while having p normal vertices in the second set (labeled from $v+m+1$ to $v+m+p$) — see Fig. 7. All vertices behave as before, see Eq. (3.2) and Eq. (3.4). Special vertices are phase-shifting and purely reflective. Normal vertices are of Grover type, however the coefficients t and r are now different for the two sets. For the transmission and reflection coefficients for normal vertices in the first set we have:

$$t_0 = \frac{2}{p} \qquad r_0 = 1 - t_0 = \frac{p-2}{p}$$

and for normal vertices in the second set:

$$t = \frac{2}{v+m} \qquad r = 1 - t = \frac{v+m-2}{v+m}.$$

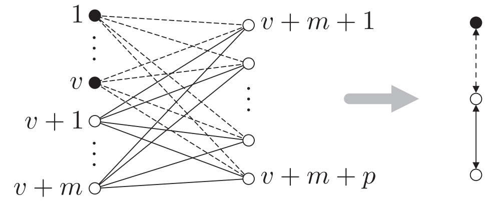

FIG. 7: A bipartite graph with v special vertices (black circles) and m normal vertices (white circles) in the first set and p normal vertices in the second set. As before, the problem reduces to a four-dimensional problem due to the existence of four subspaces invariant under the action of $\hat{U}$, as depicted on the right-hand side of the figure.

Now, the the group of automorphisms, $\mathcal{A}$, of the graph consist of all permutations of the vertices within each group (a group of special vertices in the first set and two groups of normal vertices in each set). This gives a subspace S with four orthogonal vectors corresponding to four invariant subspaces of $\mathcal{H}_G$ that span it:

$$\begin{aligned} |w_1\rangle &= \frac{1}{\sqrt{vp}} \sum_{a=1}^{p} \sum_{b=1}^{v} |v+m+a, b\rangle; \\ |w_2\rangle &= \frac{1}{\sqrt{vp}} \sum_{a=1}^{v} \sum_{b=1}^{p} |a, v+m+b\rangle; \\ |w_3\rangle &= \frac{1}{\sqrt{mp}} \sum_{a=1}^{m} \sum_{b=1}^{p} |v+a, v+m+b\rangle; \\ |w_4\rangle &= \frac{1}{\sqrt{mp}} \sum_{a=1}^{p} \sum_{b=1}^{m} |v+m+a, v+b\rangle. \end{aligned}$$

These are respectively equal superpositions of edge states that enter the group of special vertices, that leave the group of special vertices, that leave the group of normal vertices in first set and that enter this group, respectively.

The evolution is described by matrix $\hat{U}$ by the following set of evolutionary equations:

$$\begin{aligned} \hat{U}|w_1\rangle &= e^{i\phi}|w_2\rangle; \\ \hat{U}|w_2\rangle &= [-r + t(v-1)]|w_1\rangle + t\sqrt{vm}|w_4\rangle; \\ \hat{U}|w_3\rangle &= t\sqrt{vm}|w_1\rangle + [-r + t(m-1)]|w_4\rangle; \\ \hat{U}|w_4\rangle &= |w_3\rangle. \end{aligned}$$

We may notice that the problem does not depend on p — the number of normal vertices in the second set. This is a consequence of the fact, that p is important only within coefficients t_0 and r_0. These are present only in the evolution equation for state $|w_4\rangle$ where their common effect reduces to just a pure reflection with no phase-shift. The dependence on p is interesting also in the classical case where normal search on vertices would depend on p (and p may be much larger than v or m) and so classical search on edges would then be more effective, since it does not depend on p also in the classical case. The probability of finding one of the special vertices is $P = (vp)/(mp) = v/m$ and so the average number of steps is equal to m/v. We see that the structure of the graph may play an important role also in the classical case.

The matrix $\hat{U}_S$, a restriction of $\hat{U}$ to subspace S, can now written in form

$$\hat{U}_S = \begin{pmatrix} 0 & -q & s & 0 \\ \mathrm{e}^{\mathrm{i}\phi} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & s & q & 0 \end{pmatrix}, \tag{5.1}$$

where

$$\begin{aligned} q &= r - t(v-1) \\ &= -r + t(m-1) = 1 - \frac{2v}{m+v}; \\ s &= \sqrt{1-q^2} = t\sqrt{vm}; \\ q^2 + s^2 &= 1. \end{aligned} \tag{5.2}$$

Note that for large $m \gg v$ we get $q = 1-x$ with $x \sim 1/m$ and $s \sim 1/\sqrt{m}$.

The initial state

$$|\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{2p(v+m)}} \sum_{j=1}^{v+m} \sum_{k=1}^{p} \big(|a, v+m+b\rangle + |v+m+b, a\rangle\big),$$

an equal superposition of all edge states is an eigenstate of $\hat{U}_S$ for $\phi = 0$. The interesting eigenstates for us are those having eigenvalues ± 1, namely:

$$|u_\pm\rangle = \frac{\sqrt{1-q}}{2} \begin{pmatrix} 1 \\ \pm 1 \\ \pm\sqrt{\frac{1+q}{1-q}} \\ \sqrt{\frac{1+q}{1-q}} \end{pmatrix}.$$

Then $|\psi_{\text{initial}}\rangle = |u_+\rangle$ and this is the reason for $\phi = 0$ being uninteresting from the point of view of evolution which again behaves in trivial way.

Non-trivial evolution can be observed for $\phi = \pi$ where the state of the system after n steps in the case for $|u_+\rangle = |\psi_{\text{initial}}\rangle$ as initial state leads to

$$\hat{U}_S^n |\psi_{\text{initial}}\rangle \sim \frac{1}{2\sqrt{2}} \begin{pmatrix} \sin(n+1)\eta/2 + \sin n\eta/2 \\ -\sin n\eta/2 - \sin(n-1)\eta/2 \\ \cos n\eta/2 + \cos(n-1)\eta/2 \\ \cos(n+1)\eta/2 + \cos n\eta/2 \end{pmatrix}$$

and in the case for $|u_-\rangle$ as initial state leads to

$$\hat{U}_S^n |\psi_{\text{initial}}\rangle \sim \frac{1}{2\sqrt{2}} \begin{pmatrix} \sin(n+1)\eta/2 + \sin n\eta/2 \\ \sin n\eta/2 + \sin(n-1)\eta/2 \\ -\cos n\eta/2 - \cos(n-1)\eta/2 \\ \cos(n+1)\eta/2 + \cos n\eta/2 \end{pmatrix}$$

Here, $\tan\eta = 2\sqrt{vm}/(m-v)$. The second two amplitudes of the probability for edge states with edges not connected to the special vertex are close to zero for $n \cong \pi/\eta$ in both cases. Therefore, the number of steps in the walk is $\mathcal{O}(\sqrt{m/v})$. Note that in the classical case, for a blind search on edges, as noted before, these probabilities are of the order $\mathcal{O}(m/v)$, so they are quadratically larger. If we would consider a classical search on vertices (either blind or with memory), the average number of steps in such search would be $\mathcal{O}((m+p)/v)$. This means that even if m is quite small in comparison with v, p might still by very large, and the algorithm would not be effective at all. Note also that the results remain qualitatively the same for initial states that are any superposition of the states $|u_\pm\rangle$.

B. General bipartite graph with special vertices in each set

Finally let us consider the most general situation for a bipartite graph. We have two sets of vertices, with N_1 vertices in set 1 and N_2 in set 2. Of the vertices in set 1, v_1 are special vertices and $p_1 = N_1 - v_1$ are normal vertices, and in set 2, v_2 are special vertices and $p_2 = N_2 - v_2$ are normal vertices — see Fig. 8. The action of the unitary operator, $\hat{U}$ acting on a state entering a normal vertex in set 1 is given by Eq. (3.2) with[19]

$$t_1 = \frac{2}{N_2} \qquad r_1 = \frac{N_2 - 2}{N_2}, \tag{5.3}$$

and if it acts on a state entering a normal vertex in set 2 its action is again given by Eq. (3.2) but with

$$t_2 = \frac{2}{N_1} \qquad r_2 = \frac{N_1 - 2}{N_1}. \tag{5.4}$$

The action of $\hat{U}$ on a state entering a special vertex is given by Eq. (3.4). We shall number the vertices in set 1 as 1 through N_1 and those in set 2 as $N_1 + 1$ through $N_1 + N_2$. In analyzing the walk, we can, without loss of generality, assume that vertices 1 through v_1 in set 1 are special, and vertices $N_1 + 1$ through $N_1 + v_2$ are special.

There are now eight invariant subspaces, two of which, consisting of edges that connect the sets of special vertices, decouple from the rest, so our problem is essentially six-dimensional: define the following vectors

$$\begin{aligned} |w_{01}\rangle &= \frac{1}{\sqrt{v_1 v_2}} \sum_{j=1}^{v_1} \sum_{k=N_1+1}^{N_1+v_2} |k, j\rangle \\ |w_{02}\rangle &= \frac{1}{\sqrt{v_1 v_2}} \sum_{j=1}^{v_1} \sum_{k=N_1+1}^{N_1+v_2} |j, k\rangle. \end{aligned} \tag{5.5}$$

The vector $|w_{01}\rangle$ is a superposition of states leaving special vertices in set 2 and entering special vertices in set 1, and $|w_{02}\rangle$ is a superposition of edge states leaving special vertices in set 1 and entering special vertices in set 2. We have that $\hat{U}|w_{01}\rangle = \exp(i\phi)|w_{02}\rangle$ and $\hat{U}|w_{02}\rangle = \exp(i\phi)|w_{01}\rangle$, so that these vectors decouple from the rest of the problem.

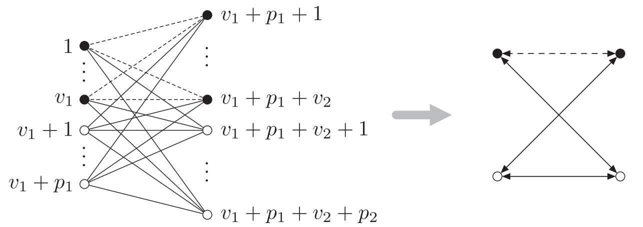

FIG. 8: General bipartite graph having v_1 special (black circles) and p_1 normal (white circles) vertices in the first set and v_2 special and p_2 normal vertices in the second set. This problem can be reduced to eight-dimensional one with two-dimensional decoupled subspace. Remaining 6-dimensions can be reduced to three when performing two steps at a time due to the oscillatory behavior of the walk in bipartite graphs. On the right-hand side of the figure, there is reduced representation of the problem to eight dimensions.

Now define

$$\begin{aligned} |w_{11}\rangle &= \frac{1}{\sqrt{v_1 p_2}} \sum_{j=1}^{v_1} \sum_{k=N_1+v_2+1}^{N_1+N_2} |k,j\rangle \\ |w_{12}\rangle &= \frac{1}{\sqrt{v_2 p_1}} \sum_{j=v_1+1}^{N_1} \sum_{k=N_1+1}^{N_1+v_2} |k,j\rangle \\ |w_{13}\rangle &= \frac{1}{\sqrt{p_1 p_2}} \sum_{j=v_1+1}^{N_1} \sum_{k=N_1+v_2+1}^{N_1+N_2} |k,j\rangle. \end{aligned} \tag{5.6}$$

These vectors consist of different sets of edge states entering set 1. Let us denote their span by S_1. Now define the vectors

$$\begin{aligned} |w_{21}\rangle &= \frac{1}{\sqrt{v_1 p_2}} \sum_{j=1}^{v_1} \sum_{k=N_1+v_2+1}^{N_1+N_2} |j,k\rangle \\ |w_{22}\rangle &= \frac{1}{\sqrt{v_2 p_1}} \sum_{j=v_1+1}^{N_1} \sum_{k=N_1+1}^{N_1+v_2} |j,k\rangle \\ |w_{23}\rangle &= \frac{1}{\sqrt{p_1 p_2}} \sum_{j=v_1+1}^{N_1} \sum_{k=N_1+v_2+1}^{N_1+N_2} |j,k\rangle. \end{aligned} \tag{5.7}$$

These vectors consist of different sets of edge states entering set 2. We shall denote their span by S_2.

Now let us consider the action of the unitary operator that advances the walk one step on these states. We find that

$$\begin{aligned} \hat{U}|w_{11}\rangle &= e^{i\phi}|w_{21}\rangle \\ \hat{U}|w_{12}\rangle &= [t_1(v_2-1)-r_1]|w_{22}\rangle + t_1\sqrt{v_2 p_2}|w_{23}\rangle \\ \hat{U}|w_{13}\rangle &= [t_1(p_2-1)-r_1]|w_{23}\rangle + t_1\sqrt{v_2 p_2}|w_{22}\rangle, \end{aligned} \tag{5.8}$$

and

$$\begin{aligned} \hat{U}|w_{21}\rangle &= [t_2(v_1-1)-r_2]|w_{11}\rangle + t_2\sqrt{v_1 p_1}|w_{13}\rangle \\ \hat{U}|w_{22}\rangle &= e^{i\phi}|w_{12}\rangle \\ \hat{U}|w_{23}\rangle &= [t_2(p_2-1)-r_2]|w_{13}\rangle + t_2\sqrt{v_1 p_1}|w_{11}\rangle. \end{aligned} \tag{5.9}$$

From these equations, we see that $\hat{U}$ maps S_1 into S_2 and vice versa. This also implies that $\hat{U}^2$ maps S_1 into itself and S_2 into itself. Therefore, if we consider a walk with an even number of steps, our six-dimensional problem turns into two three-dimensional ones. This is what we shall do.

We shall look in detail at what happens in S_2; the case of S_1 is similar. We shall only consider the case $\phi = \pi$. First, let us define the quantities

$$\begin{aligned} q_1 &= -r_1 + t_1(v_2-1) \quad s_1 = t_1\sqrt{v_2 p_2} \\ q_2 &= -r_2 + t_2(v_1-1) \quad s_2 = t_2\sqrt{v_1 p_1}, \end{aligned} \tag{5.10}$$

and note that $q_j^2 + s_j^2 = 1$ for $j = 1, 2$. If we denote $\hat{U}^2$ restricted to S_2 by $\hat{M}$, then the matrix for $\hat{M}$ in the basis $|w_{21}\rangle$, $|w_{22}\rangle$, and $|w_{23}\rangle$ is

$$M = \begin{pmatrix} -q_2 & 0 & -s_2 \\ s_1 s_2 & -q_1 & -q_2 s_1 \\ -q_1 s_2 & -s_1 & q_1 q_2 \end{pmatrix}. \tag{5.11}$$

In finding the eigenvalues and eigenvectors of this matrix, we assume that the number of special vertices is small, that is $(v_1/N_1) \ll 1$ and $(v_2/N_2) \ll 1$. In addition, we set $x_1 = 2v_1/N_1$ and $x_2 = 2v_2/N_2$. The eigenvalues and eigenvectors then are $\lambda_0 = 1$ with eigenvector

$$|\gamma_0\rangle = \frac{1}{\sqrt{2(x_1+x_2)}} \begin{pmatrix} \sqrt{2x_2} \\ \sqrt{2x_1} \\ -\sqrt{x_1 x_2} \end{pmatrix}, \tag{5.12}$$

and

$$\lambda_\pm = e^{\pm i\theta} \cong 1 \pm i\sqrt{2(x_1+x_2)}, \tag{5.13}$$

with eigenvectors

$$|\gamma_\pm\rangle = \frac{1}{\sqrt{2(x_1+x_2)}} \begin{pmatrix} \sqrt{2x_1} \\ -\sqrt{2x_2} \\ \mp i\sqrt{2(x_1+x_2)} \end{pmatrix}, \tag{5.14}$$

respectively. The angle θ is given by

$$\tan\theta = \sqrt{2(x_1+x_2)}. \tag{5.15}$$

Note, that in these equations, only the terms of lowest order in (v_1/N_1) and (v_2/N_2) have been kept.

For the initial state of our walk, we will choose the state that is an equal superposition of all edge states entering set 2. It can be expressed as

$$\begin{aligned} |\psi_{\text{initial}}\rangle = \frac{1}{\sqrt{N_1 N_2}} (&\sqrt{v_1 v_2}|w_{02}\rangle + \sqrt{v_1 p_2}|w_{21}\rangle \\ &+ \sqrt{v_2 p_1}|w_{22}\rangle + \sqrt{p_1 p_2}|w_{23}\rangle). \end{aligned} \tag{5.16}$$

This vector is not entirely in S_2, but its component that is not in S_2 is small, and it stays small throughout the evolution. Neglecting this small component, we find that

$$\hat{U}^{2n}|\psi_{\text{initial}}\rangle = \begin{pmatrix} -\sqrt{x_1/(x_1+x_2)}\sin(2n\theta) \\ \sqrt{x_2/(x_1+x_2)}\sin(2n\theta) \\ -\cos(2n\theta) \end{pmatrix}. \tag{5.17}$$

From this equation, we see that, when

$$2n = \frac{\pi}{2\theta} = \frac{\pi}{2\sqrt{2(x_1 + x_2)}}, \tag{5.18}$$

we are with certainty on an edge connected to a special vertex. If after this many steps we measure the particle to determine which edge it is on, with probability $x_1/(x_1 + x_2)$ we find it on an edge connected to a special vertex in set 1, and with probability $x_2/(x_1 + x_2)$ we find it on an edge connected to a special vertex in set 2.

In order to get a better feel for this solution, let us consider the case $v_1 = v_2 = 1$. In that case

$$\theta = 2\left(\frac{1}{N_1} + \frac{1}{N_2}\right)^{1/2}. \tag{5.19}$$

When $2n = \pi/2\theta$, the probability of finding the particle on an edge connected to the special vertex in set 1 is $N_2/(N_1 + N_2)$ and the probability of being on an edge connected to the special vertex in set 2 is $N_1/(N_1 + N_2)$. Now suppose that $N_2 \gg N_1$. How many steps would it take to find the special vertices in each of the sets? We find that the number of steps in the walk is $\pi/2\theta \sim \sqrt{N_1}$. The number of times the walk would have to be repeated in order find the special vertex in set 1 is $\mathcal{O}(1)$, while the number of times to find the special vertex in set 2 is $\mathcal{O}(N_2/N_1)$. Therefore, the total number of steps to find the special vertex in set 1 is $\mathcal{O}(\sqrt{N_1})$, and the total number of steps to find the special vertex in set 2 is $\mathcal{O}(N_2/\sqrt{N_1})$. A classical search would require $\mathcal{O}(N_1)$ steps to find the special vertex in set 1 and $\mathcal{O}(N_2)$ steps to find the special vertex in set 2.

VI. CONCLUSION

We have considered several cases of highly symmetric (complete and bipartite) graphs with several special vertices and scattering quantum walks on them. The symmetry of these graphs leads to a reduction in dimensionality of the problem from roughly N^2 to three or four. For both types of graphs, we were able to find a quadratic speedup over the classical search. These results were obtained by taking the phase-shift of special vertices to be π. Taking $\phi = 0$ results in a trivial evolution, with constant probabilities of finding the particle in any edge state. In this case quantum walks reduce to the classical blind search on edges. In this sense, quantum search reaches its classical counterpart. When this happens, the classical search on vertices with memory is faster.

We have also studied the change in behavior when changing the phase-shift ϕ for a complete graph with one special vertex. While for $\phi = \pi$ we have a non-trivial behavior suitable for searches in these graphs, for $\phi = 0$ we get only a static case. Cases between these values were explored numerically. As a measure for suitable comparison between different choices of ϕ, we chose the average number of steps that need to be taken to successfully find the special vertex. We noticed that the quantum algorithm is always at least as fast as its classical counterpart.

Finally we note, that the approach used here is isomorphic to the one used in Ref. [11], where a search on a hypercube was studied. There is presented an algorithm for finding the special vertex with probability approximately 1/2 which is in contrast with our findings of the probability being close to one. This is due to the fact, that in our case this probability is (almost) equally split between two possible cases for positions of the special vertex on selected edge. This, in the case of Ref. [11] corresponds to either finding particle on the special vertex or finding it on the neighboring vertex with coin pointing to the special one — they discard this type of states as an unsuccessful search. Similar findings have been also found in Ref. [18].

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