Quantum walk-based search and symmetries in graphs

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Abstract

In this paper we present a lemma, which helps us to establish a link between the distribution of success probabilities from quantum walk based search and the symmetries of the underlying graphs. With the aid of the lemma, we identified certain graph structures of which the quantum walk based search provides high success probabilities at the marked vertices. We also observed that many graph structures and their vertices can be classified according to their structural equivalence using the search probabilities provided by quantum walks, although this method cannot resolve all non-equivalent vertices for strongly regular graphs.

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1 Introduction

Quantum walks are the quantum analogue of classical random walks. It has received much attention recently due to its applicability as a computational model in quantum computation [1, 7, 15, 10], as well as a wide range of potential applications [17, 8, 18, 12, 5, 16, 19]. In particular, the application of quantum walks in developing search algorithms is noteworthy [22, 2, 9, 3, 14, 11, 20, 13]. It has been observed that in a quantum walk based search, where one or more vertices are marked with a different coin operator, the topology of the database is crucial in determining its search efficiency. Therefore, given an underlying graph, it is an important question to ask how successful a quantum walk-based search would be. In reference [4], topological facts such as symmetry and centrality of the marked element have been studied, and some graph structures that give efficient search results were identified. Our objective in this work is to generalise the relation between the success probabilities and the topology of the graph, and to identify suitable graph structures for quantum walk-based search, by their topology.

The paper is organised as follows: Section 2 provides an introduction to quantum walk-based search over a graph. Section 3 describes the lemma that explains the distribution of success probabilities of quantum walk based search over a graph. In Section 4 we discuss quantum search results on complete graphs and complete bipartite graphs. In the same section, we give clues to determine if a graph is suitable for quantum walk-based search, by considering its topology. In Section 5, we apply the lemma discussed in section 3 to partition many graphs by their vertex equivalence classes. Section 6 contains our conclusions.

2 Quantum walk-based search over a graph

A graph $G = (V, E)$ is a pair of sets, where V is non-empty and each element of E is a set of two distinct elements of V. The elements of V are called vertices, and the elements of E are called the edges drawn between two distinct vertices. The discrete-time quantum walk takes place in the Hilbert space $\mathcal{H}_{\mathcal{P}} \otimes \mathcal{H}_{\mathcal{C}}$ [4, 22], where $\mathcal{H}_{\mathcal{P}}$ is the position Hilbert space spanned by an orthonormal set of vertex states $\{|v_i\rangle : i = 1, 2, \ldots, n\}$, $\mathcal{H}_{\mathcal{C}}$ is the coin Hilbert space spanned by an orthonormal set of coin states $\{|c_j\rangle^i : j = 1, 2, \ldots, d_i\}$, and d_i is the degree of vertex v_i. If v_i and v_j are adjacent vertices, then the subvertex state $|v_i, c_j\rangle$ corresponds to the directed edge (v_i, v_j) at vertex v_i. The quantum walk on a graph is the repeated application of the unitary time-evolution operator $\hat{U} = \hat{S} \cdot \hat{C}$, where S is the shift operator acting on the extended space $\mathcal{H_P} \otimes \mathcal{H_C}$ as $S|v_i, c_j\rangle = |v_j, c_i\rangle$, and $\hat{C}$ is the *global* coin operator defined as an $n \times n$ block diagonal matrix

$$\hat{C} = \begin{pmatrix} \ddots & 0 & 0 & 0 & 0 \\ 0 & \hat{\mathcal{C}}^{i-1} & 0 & 0 & 0 \\ 0 & 0 & \hat{\mathcal{C}}^{i} & 0 & 0 \\ 0 & 0 & 0 & \hat{\mathcal{C}}^{i+1} & 0 \\ 0 & 0 & 0 & 0 & \ddots \end{pmatrix}, \tag{1}$$

with each $d_i \times d_i$ block $\hat{\mathcal{C}}^i$ denoting the *local* coin operator acting on vertex v_i, defined as

$$\hat{\mathcal{C}}^i_{k,l} = \begin{cases} -\delta_{kl} & \text{if } v_i = v_m, \text{ the searched-for vertex} \\ -\delta_{kl} + 2/d_i & \text{otherwise} \end{cases} \tag{2}$$

for $k, l \in 1, 2, \ldots, d_i$ [21]. In such a quantum walk based search scheme, we apply a distinct coin operation at the marked vertex that changes its phase by 90 degrees. This alteration propagates to other vertices through the shifting operator in the form of probability amplitudes interpretable as wave-like interference.

The quantum walker is initially assumed to be in an equal superposition of all subvertex states, i.e.

$$|\Psi_0\rangle = \frac{1}{\sqrt{n}} \sum_{i=1}^{n} \sum_{j=1}^{d_i} \frac{1}{\sqrt{d_i}} |v_i, c_j\rangle . \tag{3}$$

The success probability $P_s(t)$ is defined as the probability of finding the walker at the marked vertex v_m at time t, given by

$$P_s(t) = \sum_{j=1}^{d_m} |\langle v_m, c_j \mid \Psi(t)\rangle|^2 , \tag{4}$$

where $|\Psi(t)\rangle = (\hat{S} \cdot \hat{C})^t |\Psi_0\rangle$ and t represents the number of time steps.

3 Quantum walk-based search and equivalence classes

On graph theoretic properties, global symmetry relations are of our particular interest. These symmetries are defined in terms of graph automorphisms. The automorphism group of a graph G is the group formed by all structure-preserving permutations of its vertices, and is denoted by $aut(G)$. Two vertices u and v in G are said to be structurally equivalent if there is an automorphism σ in $aut(G)$ such that $\sigma(u) = v$. Therefore, $aut(G)$ is a permutation group. The orbit of an element in a permutation group is defined as follows: If Γ is a permutation group on Ω, the orbit of the element α in Ω is defined as its image under Γ. i.e. $\Gamma(\alpha) = \{\varphi(\alpha) : \varphi \in \Gamma\}$. A permutation group Γ is said to be transitive if there is some α in Γ so that $\Gamma(\alpha) = \Omega$. A graph is said to be vertex-transitive, if all its vertices are structurally equivalent. It is an immediate consequence of the definition that the transitivity of the automorphism group is equivalent to the vertex transitivity of the graph. Thus, a graph can be tested for vertex transitivity by its associated automorphism group.

On quantum walk based search over a graph, we establish the following relation:

Lemma 1. *In the quantum walk based search over a connected graph G with vertex v_m marked as described above, provided all vertices adjacent to v_m are structurally equivalent, all structurally equivalent vertices in $G - v_m$ that are non-adjacent to v_m in the original graph G produce identical success probabilities. Here, $G - v_m$ is the graph obtained by removing v_m and all its incident edges from G.*

Proof. Let u_1, u_2, $\ldots$, u_k be the vertices adjacent to the marked vertex v_m and structurally equivalent in G. The phase inverted alteration to the amplitudes of subvertex states $\{|v_m, c_j\rangle : j = 1, 2, \ldots, d_m\}$, due to the special coin operator at v_m, is propagated to u_1, u_2, $\ldots$, u_k by the shift operation. Since u_1, u_2, $\ldots$, u_k have the same structural relationship with v_m in graph G, the amplitudes assigned to them by the coin and shift operations are exactly the same. Now take two vertices v_1 and v_2 that are not adjacent to v_m in the original graph G, but structurally equivalent in $G - v_m$. Since G is a connected graph, both v_1 and v_2 would have to be connected to the vertex set u_1, u_2, $\ldots$, u_k via a sequence of edges. Due to the structural equivalence of v_1 and v_2 in $G - v_m$, every path connecting v_1 and u_i ($i = 1, 2, ..., k$) has an equivalent path connecting v_2 and u_j for some $j \in 1, 2, ..., k$. The propagation of the phase inverted alteration at v_m is clearly identical along equivalent paths. Consequently, v_1 and v_2 produce identical success probabilities. $\square$

The importance of the above relation is that the vertices of a graph can be classified by the success probability defined by Eq. 4 in the following manner: the marked vertex v_m, vertices adjacent to v_m, and groups of structurally equivalent vertices in $G - v_m$. The first in the above classification is the marked vertex itself. Highly distinguishable success probabilities at the marked vertex v_m are often expected due to the action of a marker at this vertex. The second class is formed by the vertices adjacent to the marked vertex, which often have sufficiently high success probabilities, especially when they are structurally equivalent in G. The groups of structurally equivalent vertices in $G - v_m$ would have the same success probabilities within their respective groups, provided all vertices adjacent to v_m are structurally equivalent. This leads to the classification of the 3rd, 4th, etc classes.

As an example, we consider the Pappus graph which is one of 12 graph structures with cubic regularity and distance transitivity. A graph is said to be distance transitive if any two pairs of vertices which are at the same distance apart behave in the same way, where the distance is the size of the shortest path between two vertices. Distance transitivity is a higher level of symmetry that immediately implies vertex transitivity, and thus the Pappus graph is considered to have a high degree of symmetry

The vertices of Pappus graph are labelled v_1, v_2,$\ldots$,v_{18}, as illustrated in Figure 1. We can categorise these vertices into four classes by their success probabilities. The marked vertex v_1 has produced a distinguishably high probability pattern that is not followed by any other vertex. A second class is formed by the three vertices v_2, v_8, and v_{18}, which are adjacent to v_1 and structurally equivalent in G. Consequently, according to Lemma 1, structurally equivalent vertices in $G - v_1$ produce identical success probabilities, as shown in Figure 2. Such properties can be used to partition the rest of the vertex set in G into equivalence classes. For example, the vertices v_4, v_5, v_6, v_{10}, v_{12}, v_{14}, v_{15} and v_{16} possess the same success probability and they form the third class. A different success probability pattern is observed at vertices v_3, v_7, v_9, v_{11}, v_{13} and v_{17} to form the fourth class. In summary, the quantum walk based search procedure has partitioned the vertex set in G into the structural equivalence classes.

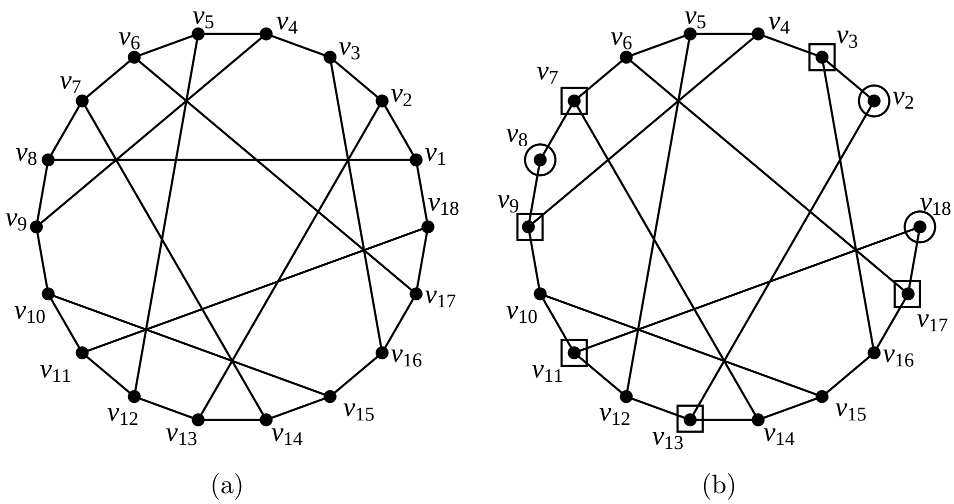


Figure 1: (a) Pappus graph; (b) Structurally equivalent vertices in $G - v_m$, grouped by dots, circle-dots, and square-dots.

However, this scheme only works when both conditions of Lemma 1 are satisfied. As an example, if the vertices adjacent to the marked vertex v_m are not structurally equivalent in G, then the success probability may be very different even for structurally equivalent vertices in $G - v_m$, as illustrated by v_1 and v_8 in Figure 3 and 4.

4 Quantum walk-based search and symmetries in graphs

4.1 Complete graphs

A graph with n vertices and the maximum number of edges is called a complete graph denoted by K_n. The quantum walk based search over the complete graph K_n is the most successful out of all graphs on n vertices, since it minimises the diversity of the vertices adjacent to the marked vertex. It is seen instantly that the adjacency factor is neutralised as the marked vertex is adjacent to all other vertices. And, the removal of this vertex from K_n results in K_{n-1}, again a graph with the highest degree of symmetry. In this case, there are exactly two classes in the probability distribution: the marked

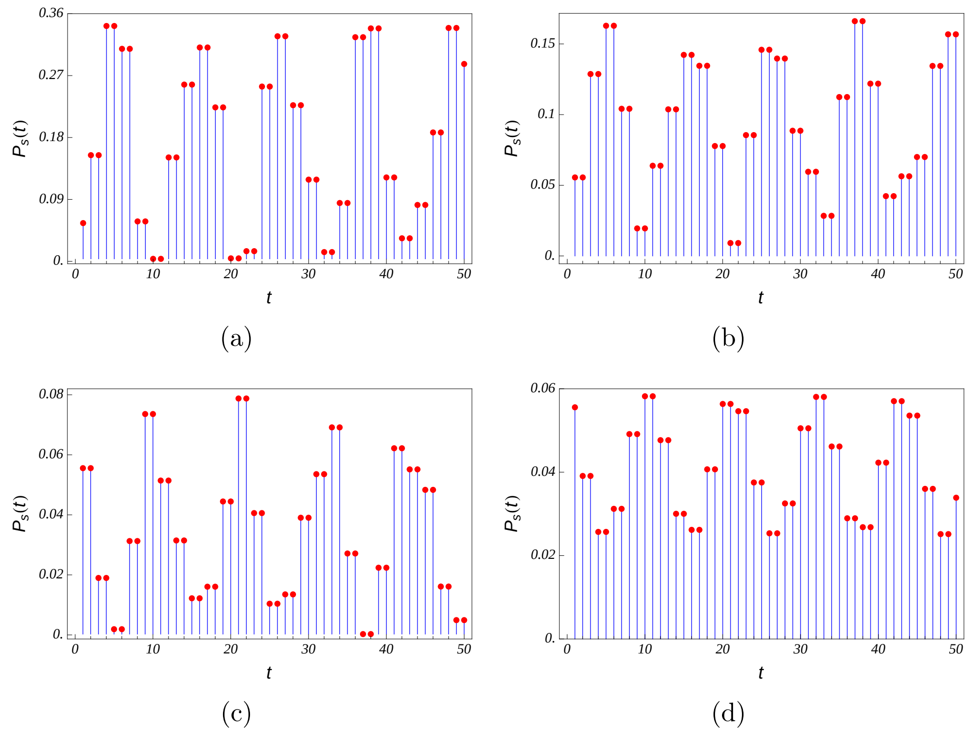
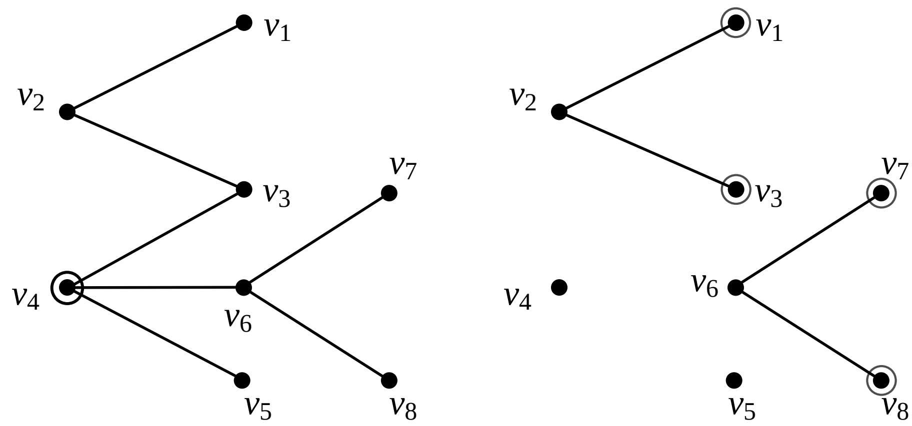


Figure 2: Success probabilities at vertices (a)v_1; (b)v_2, v_8, v_{18}; (c)v_4, v_5, v_6, v_{10}, v_{12}, v_{14}, v_{15}, v_{16}; and (d) v_3, v_7, v_9, v_{11}, v_{13}, v_{17} of the Pappus graph.

vertex and all other vertices. As a result, the marked vertex can be clearly distinguished from the other vertices, making the search successful. Figure 5 shows the search results on K_{10} with vertex v_1 marked, which has a much higher search probability than the other vertices.

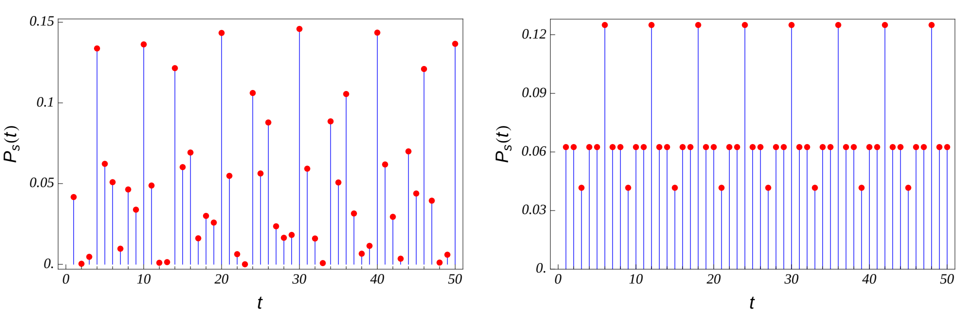
4.2 Complete bipartite graphs

A graph is said to be bipartite if the vertex set is partitioned into two subsets, each subset having no internal edges. The complete bipartite graph denoted by $K_{m,n}$ is the bipartite graph on partitions with m and n vertices so that each vertex in a partition is adjacent to all vertices in the other partition, as shown in Figure 6. If $m > n$, we refer vertex in the partition with n vertices as a higher degree vertex, and a vertex in the other partition as a lower degree vertex. Quantum search on complete bipartite graphs were



(a) (b)

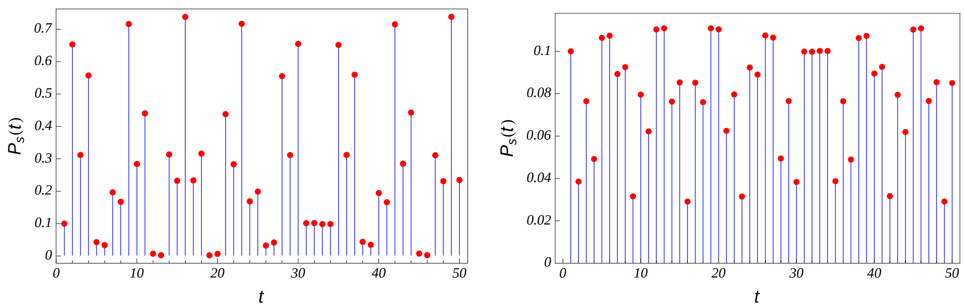
Figure 3: (a) An example graph G with v_4 marked; (b) four structurally equivalent vertices v_1, v_3, v_7 and v_8 in $G - v_4$.



(a) (b)

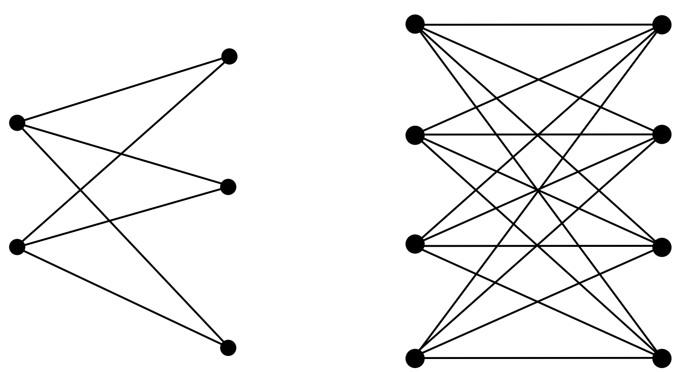
Figure 4: (a) and (b) success probabilities at the two structurally equivalent vertices v_1 and v_8 in $G - v_4$. Here, G is the example graph shown in Figure 3.

of particular interest. The searches can be categorised as higher degree vertex marked (HDVM) and lower degree vertex marked (LDVM). Our observations of HDVM search suggest that the search becomes most successful on $K_{m,n}$ when $m = 1$. Thus, $K_{1,n}$ is recommended as a highly suitable graph structure for quantum walk based search. We have observed the probability amplitudes for HDVM search on $K_{m,n}$ for fixed n and m=1,2,. . . ,n. Though the search on



(a) (b)

Figure 5: Success probabilities in quantum search on K_{10} at (a) the marked vertex and (b) all other non-marked vertices



(a) (b)

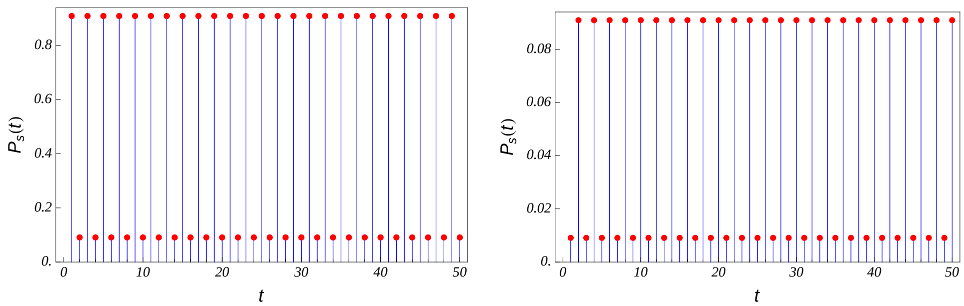
Figure 6: Two complete bipartite graphs: (a)$K_{2,3}$ and (b) $K_{4,4}$

$K_{1,n}$ was successful, $K_{2,n}$ gives the most unsuccessful search result amongst all complete bipartite graphs for HDVM search. In general, the two higher degree vertices exhibit the same pattern for quantum search despite the fact that only one of these vertices is marked. When the index m increases from 3, the success of the search starts to increase gradually. A considerably successful search result is obtained at $m = n$.

Figure 7 shows the success of HDVM search on $K_{1,10}$. The maximum success probability at the marked vertex is significantly higher than that at the low degree vertex. Removal of the higher degree vertex from $K_{1,n}$ results the null graph on n vertices. The null graph is highly symmetric and also the adjacency factor is uniform on all these n vertices. Therefore, the search is expected to be successful on $K_{1,n}$. Also it is the complete bipartite graph in which a high degree of symmetry is achieved due to the removal of the marked vertex. The variation of the success of HDVM search with m on $K_{m,10}$ is depicted in Figures 8, 9 and 10. Maximum success probability at a non-marked vertex changes rapidly with m. Figure 11 illustrates the failure of HDVM search on $K_{2,m}$. In particular, for $K_{2,3}$, the success probabilities at the marked vertex is exactly the same as the ones at the non-marked vertex as shown in Figure 11(a) and 11(b). Consequently, the search procedure would not be able to distinguish the marked vertex. For $K_{2,4}$ and $K_{2,10}$, the maximum success probability at the marked vertex is too low to be a useful measure, as shown in Figure 11(c) to 11(f). The results of HDVM search on $K_{m,n}$ can be summarised as follows: (1) HDVM quantum search is highly applicable on $K_{1,n}$; (2) HDVM search fails on $K_{2,n}$; (3) the success of the HDVM search is monotonically increased with the index i on $K_{i,n}$ for i=3,4,...,n.

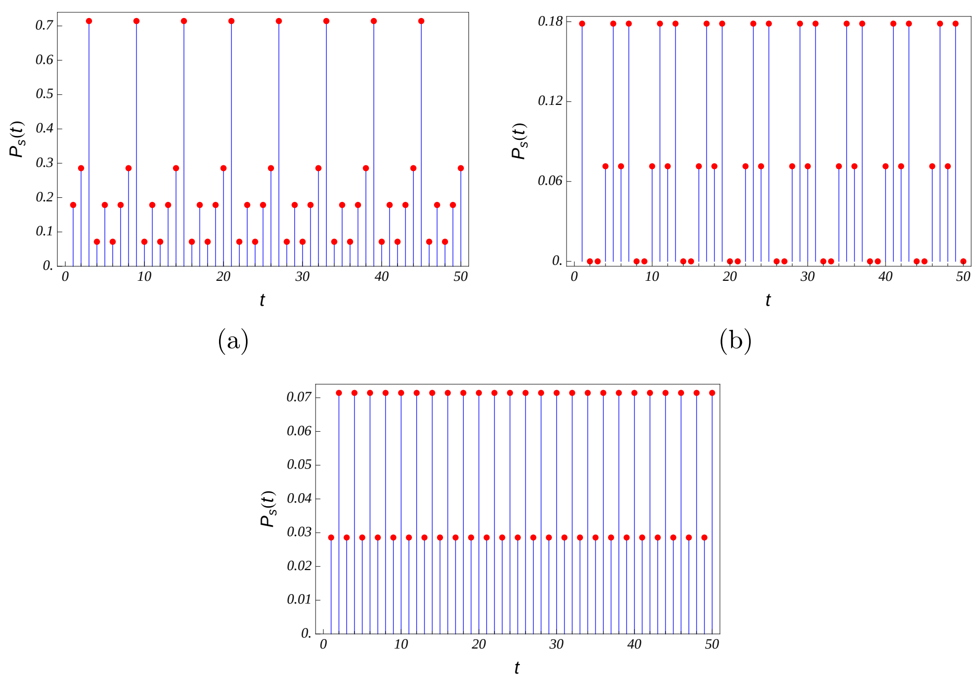
When the HDVM search on $K_{m,n}$ for m=3,4,...,n is considered, note that the effect on symmetry after removing a higher degree vertex is decreasing with m. As the adjacency factor and the equivalence factor overlap at lower degree vertices, only three classes of probability amplitudes will occur. The probability amplitudes at the higher degree vertices other than the marked vertex are decreasing with i. Therefore, a considerably successful search is performed on the regular complete bipartite graph $K_{n,n}$. On the other hand, $K_{2,n}$ is the complete bipartite graph in which the symmetry is most affected due to the removal of the marked vertex in HDVM search, leading to an unsuccessful search on this graph.

LDVM search on complete bipartite graphs does not in general achieve the success of a HDVM search, nevertheless it does not fail completely as in



(a) (b)

Figure 7: Success probabilities in HDVM quantum search over $K_{1,10}$ (a): the marked vertex; (b) all other non-marked vertices



(a) (b)

(c)

Figure 8: Success probabilities in HDVM quantum search over $K_{4,10}$: (a) marked vertex; (b) all high-degree non-marked vertices; (c) all low degree non-marked vertices.

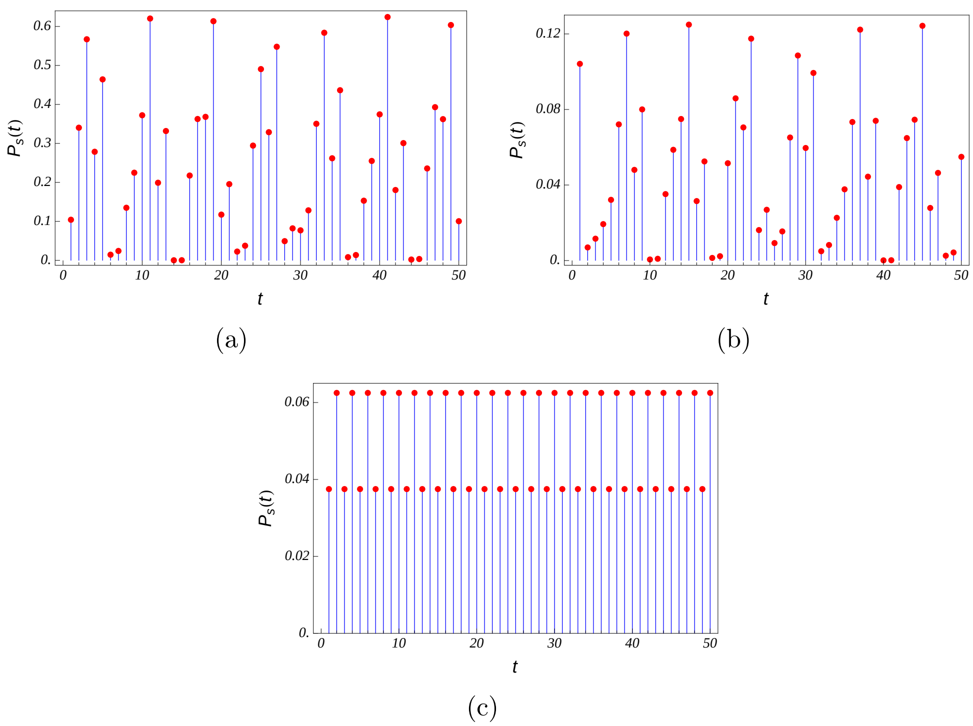


Figure 9: Success probabilities in HDVM quantum search over $K_{6,10}$: (a) marked vertex; (b) all high-degree non-marked vertices; (c) all low degree non-marked vertices.

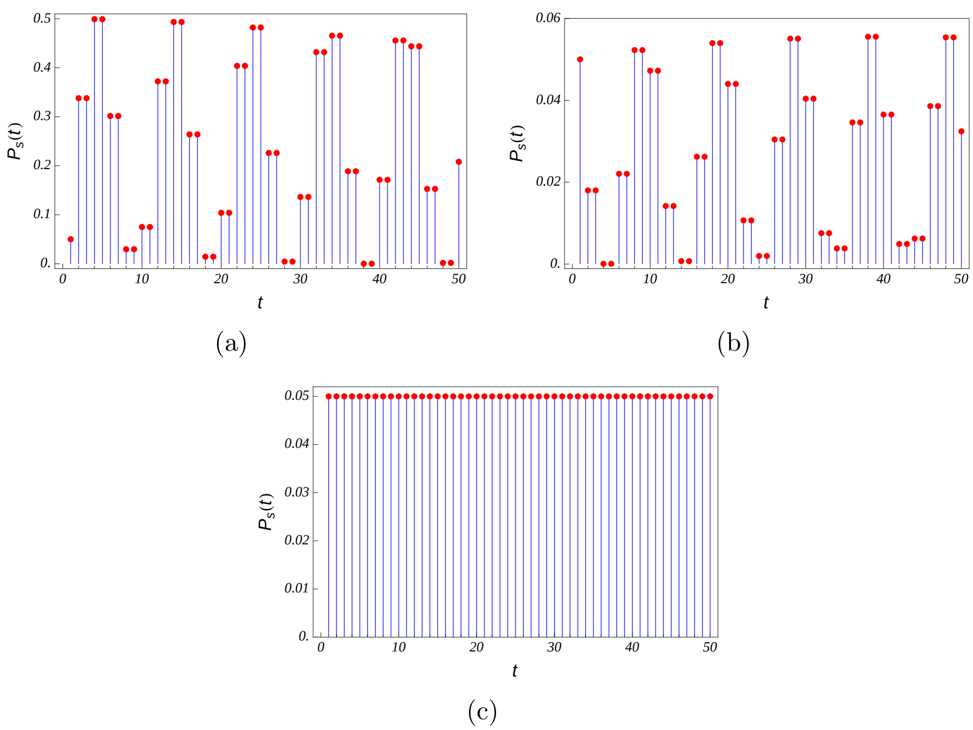


Figure 10: Success probabilities in HDVM quantum search over $K_{10,10}$ (a) marked vertex; (b) all vertices non-adjacent to the marked vertex; (c) all vertices adjacent to the marked vertex.

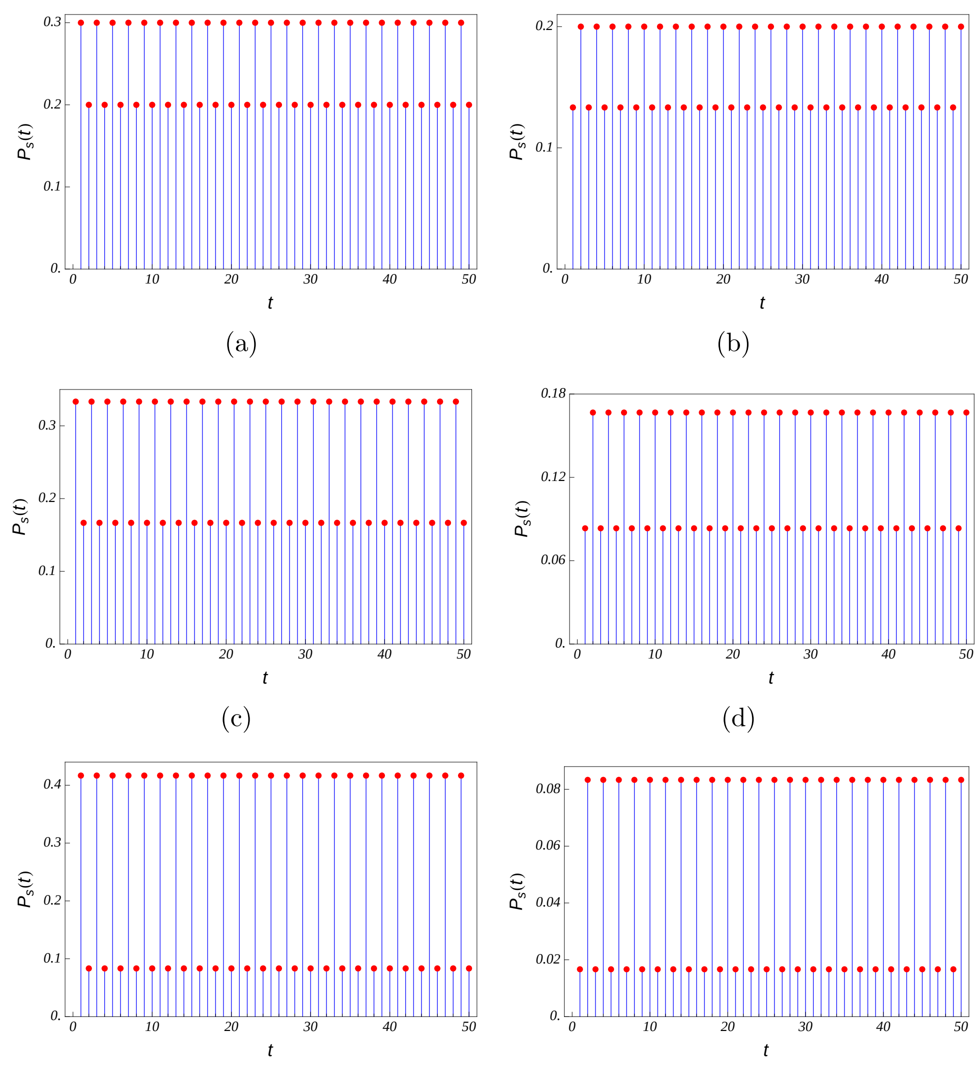
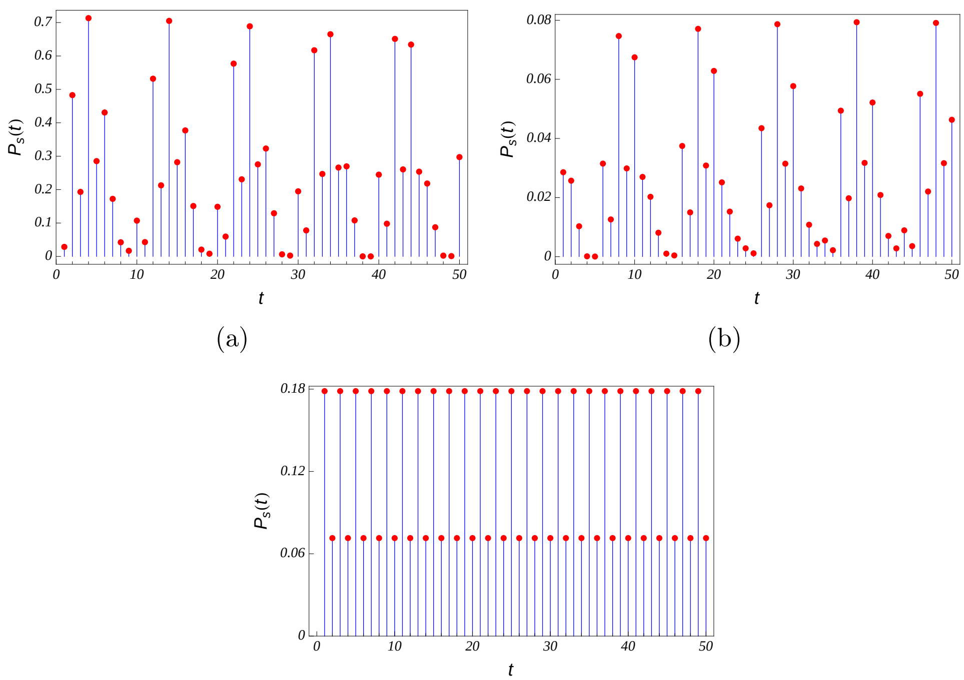


Figure 11: Success probabilities in HDVM quantum search over (a) $K_{2,3}$ at the marked and non-marked degree-3 vertex; (b) $K_{2,3}$ at all degree-2 vertices; (c) $K_{2,4}$ at the marked and non-marked degree-4 vertex; (d) $K_{2,4}$ at all degree-2 vertices; (e) $K_{2,10}$ at the marked and non-marked degree-10 vertex; (f) $K_{2,10}$ at all degree-2 vertices.



(a) (b) (c)

Figure 12: LDVM search results for $K_{4,10}$ at (a) the marked vertex (b) all non-marked degree-4 vertices and (c) all non-marked degree-10 vertices

the case of HDVM search on $K_{2,n}$. It should be noted that the adjacency and the equivalence factors describe LDVM search too. In LDVM search results, three explicit probability classes are vigilant: (1) the marked vertex, (2) high degree vertices, and (3) low degree vertices except the marked. LDVM search results on $K_{4,10}$ are depicted in Figure 12.

4.3 Cayley trees

Most widely known and extensively studied family of vertex transitive graphs are the Cayley graphs. These graphs are formed by a group G and one of its proper subsets S. The condition that must be satisfied by S are as follows: the identity element of the group must not belong to S, and if S contains an element x, its inverse x^{-1} also must be contained in S. The Cayley graph G with the connection set S is denoted by $Cay(G,S)$=(V,E), where V is the set of elements in G and $(g,h)\in E$ if and only if there exists some s in S so that $h = sg$. A Cayley graph of the free group on n generators is called an n-Cayley tree, which is a connected and acyclic graph in which each vertex of degree more than 1 has a constant number of branches. This graph can be extended to layers, and an r-generation n-Cayley tree is such a graph with r layers. A 2nd generation 3-Cayley tree is illustrated in Figure 13(a).

Berry and Wang [4] studied the relation of centrality of a vertex to its success probability in some details. In particular, they observed a close correlation between classically defined random walk centrality and the maximum quantum search probability for Cayley trees. Another measure of centrality of a vertex v in a given graph is the greatest geodesic distance between v and any other vertex, defined as [6]

$$ecc(v) = max\{dist(u, v) : u \in V(G)\}. \tag{5}$$

We observe that the quantum-walk based search on Cayley trees becomes more successful when the marked vertex has a lower eccentricity, as shown in Figure 13(b). When the central vertex (the vertex with minimum eccentricity) of a k-generation r-Cayley tree is marked, the adjacency factor is the same for all vertices in the next level. Furthermore, any two vertices non-adjacent to the central vertices taken from the same level will be structurally equivalent in $G - v_m$, and consequently they produce identical success probabilities following to Lemma 1. For the non-central vertex marked search, results on Cayley trees can also be readily explained and predicted by Lemma 1.

5 Partitioning the vertex set of a graph by quantum walk-based search

Though the quantum algorithms were originally implemented on graphs in order to search through databases, later on they were used to identify certain topological properties of that database [4]. Here, we make use of our observation to formulate a method that serves as an algorithm for partitioning a wide range of graphs according to its vertex equivalence. Suppose we are given a graph G with n vertices to be partitioned by its vertex symmetries. We add a new vertex v_m to that graph, and join it with each vertex of the graph, making its degree equal to n. The resulting graph on $n+1$ vertices is to be subjected to the quantum walk based search, where v_m is the marked

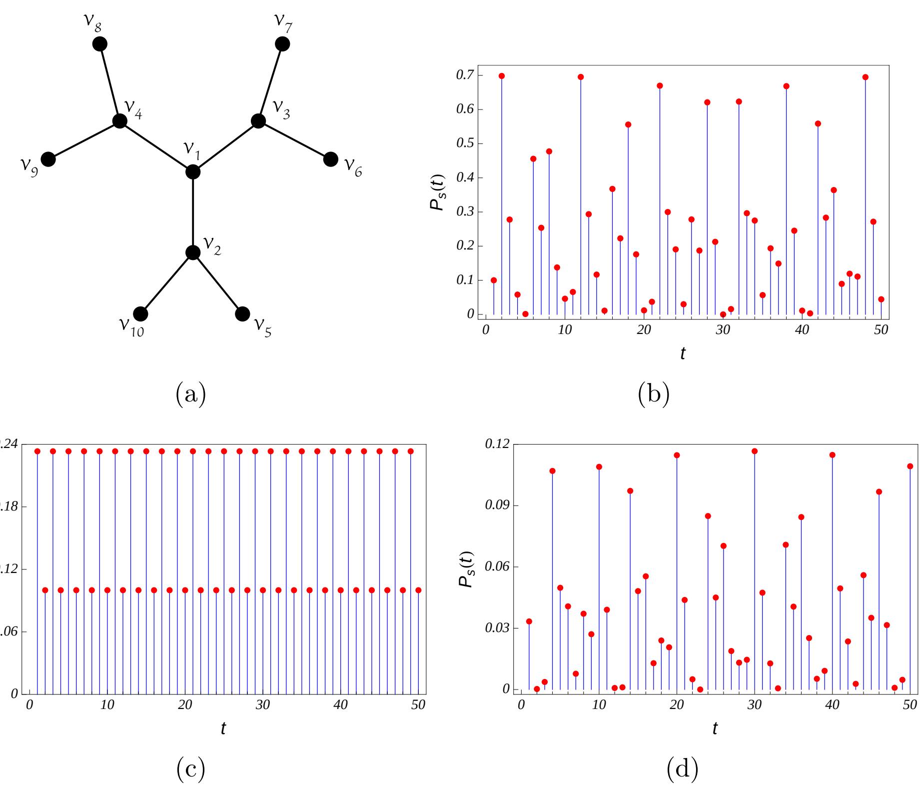


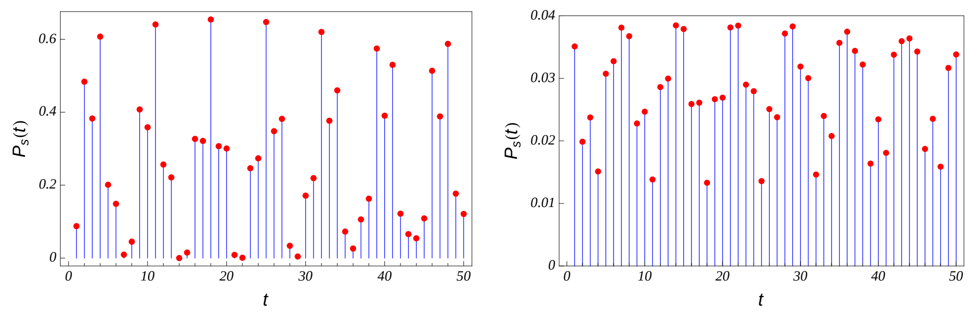
Figure 13: (a) 2nd generation 3-Cayley tree; Success probabilities at (b) the central marked vertex v_1, (c) level one vertices $\{v_2, v_3, v_4\}$, and (d) level two vertices $\{v_5, ..., v_{10}\}$

vertex. We observe that the final pattern of success probabilities are entirely determined by vertex symmetries of G, as the adjacency factor has been neutralised by joining v_m to all the vertices in G. Consequently, for graph structures and vertices satisfying the conditions imposed in Lemma 1, structurally equivalent vertices will exhibit identical success probabilities, and the graph can be readily partitioned without computing its automorphism group.

However, several researchers had observed that a single-particle quantum-walk-based algorithm fails in isomorphism testing over strongly regular graphs if no other utensil is applied to break their inherent symmetry [12]. A k-regular graph on n vertices is said to be strongly regular with parameters (n, k, λ, μ), if every pair of adjacent vertices have λ common neighbours and every pair of non-adjacent vertices have μ common neighbours. Note that certain necessary and sufficient conditions for strongly regular graphs can be derived in terms of Seidel adjacency matrices. The Seidel adjacency matrix of a graph G is defined as the matrix $A = (a_{ij})$ where $a_{jj} = 0$, $a_{ij} = -1$ if v_i and v_j are adjacent, and $a_{ij} = 1$ if v_i and v_j are non-adjacent. A graph with Seidel adjacency matrix A is said to be strong if there exist two real numbers ρ_1 and ρ_2 satisfying $(A - \rho_1 I)(A - \rho_2 I) = (n - 1 + \rho_1\rho_2)J$, where n is the number of vertices of the graph, I is the identity matrix of order n, and J is the matrix of whose elements equal to one. A graph is regular whenever there exists an integer ρ_0 so that $AJ = \rho_0 J$. Thus, a strongly regular graph is characterized by combining the above conditions. As an example, we applied the above described method to partition (by its vertex equivalence) the Paulus graphs, which are derivable from the Seidel adjacency matrix and strongly regular with parameters of $(n = 26, k = 10, \lambda = 3, \mu = 4)$. Note these graphs are not vertex transitive and none of their vertices are structurally equivalent. However, all vertices except the marked produce identical success probabilities at all time steps, as shown in Figure 14. Nonetheless, this failure does not contradict Lemma 1, namely no pair of identical vertices produce different success probabilities.

6 Discussion and conclusions

Lemma 1 can be used to predict the quantum search results over graphs with certain degree of symmetry. We have also demonstrated its applicability in classifying certain graph structures such as complete graphs and complete



(a) (b)

Figure 14: Success probabilities at (a) marked vertex and (b) all non-marked vertices of the Paulus graph with parameters (26, 10, 3, 4)

bipartite graphs according to the success of quantum search upon them. It should be noted that for any class of graphs that satisfy the conditions in the lemma, this classification holds. Also the lemma was used to partition some graphs by vertex equivalence classes.

Though strongly regular graphs obey *lemma 1*, that is any two structurally equivalent vertices in $G - v_m$ produce identical success probabilities, we have shown that structurally non-equivalent vertices may also produce identical success probabilities. Producing identical success probabilities is a necessary condition for two vertices to be structurally equivalent. However it is not a sufficient condition, as illustrated by an explicit counterexample of the Paulus graphs, which are strongly regular. It is an interesting subject for further study to reveal a necessary and sufficient condition.

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