

Influence of coin symmetry on infinite hitting times in quantum walks

Prithviraj Prabhu  and Todd A. Brun 

Ming Hsieh *Department of Electrical and Computer Engineering, University of Southern California, Los Angeles, California 90007, USA*



(Received 9 September 2021; accepted 23 February 2022; published 11 March 2022)

Classical random walks on finite graphs have an underrated property: a walk from any vertex can reach every other vertex in finite time, provided they are connected. Discrete-time quantum walks on finite connected graphs, however, can have infinite hitting times. This phenomenon is related to graph symmetry, as previously characterized by the group of direction-preserving graph automorphisms that trivially affect the coin Hilbert space. If a graph is symmetric enough (in a particular sense), then the associated quantum walk unitary will contain eigenvectors that do not overlap a set of target vertices for any coin-flip operator. These eigenvectors span the infinite-hitting-time (IHT) subspace. Quantum states in the IHT subspace never reach the target vertices, leading to infinite hitting times. However, this is not the whole story: the graph of the three-dimensional cube does not satisfy this symmetry constraint, yet quantum walks on this graph with certain symmetric coins can exhibit infinite hitting times. We study the effect of coin symmetry by analyzing the group of coin-permutation symmetries (CPSs): graph automorphisms that act nontrivially on the coin Hilbert space but leave the coin operator invariant. Unitaries using highly symmetric coins with large CPS groups, such as the permutation-invariant Grover coin, are associated with higher probabilities of never arriving, as a result of their larger IHT subspaces.

DOI: [10.1103/PhysRevA.105.032206](https://doi.org/10.1103/PhysRevA.105.032206)

I. INTRODUCTION

A classical random walk can be described by the movement of a particle on a graph, where the vertices represent possible locations and the edges connect neighboring sites. At each step, the next edge is chosen randomly [1]. Quantum walks are the unitary analogs of these classical random walks [2,3]. Similar to the classical case, there are discrete-time [4,5] and continuous-time [6,7] versions of quantum walks. In this paper, we consider only discrete-time quantum walks.

The unitary operator $\hat{U}$ corresponding to one time step in the discrete-time quantum walk can be decomposed into two parts: $\hat{U} = \hat{S}(\hat{\mathbf{1}}_v \otimes \hat{C})$. The Hilbert space of $\hat{U}$ is $\mathcal{H} = \mathcal{H}_v \otimes \mathcal{H}_c$, where $\mathcal{H}_v$ and $\mathcal{H}_c$ are the Hilbert spaces of the position (vertices) and of the internal degree of freedom (coin), respectively. The shift operator $\hat{S}$ propagates quantum states between the vertices of the graph. It is analogous to the adjacency matrix of the graph, but since the shift depends on the state of the coin, it operates on the complete Hilbert space $\mathcal{H}$. It takes the form

$$\hat{S} = \sum_{v,c} |c(v)\rangle \langle v| \otimes |c\rangle \langle c|, \quad (1)$$

where $\{|v\rangle\}$ are vertex basis states, $\{|c\rangle\}$ are coin basis states, and $|c(v)\rangle$ is the neighboring vertex to v along the edge labeled by coin state c .

The coin operator $\hat{C}$ acts on the coin Hilbert space $\mathcal{H}_c$. Discrete-time quantum walks use these operators to mix the particle's internal basis states at each vertex. A vertex with d edges (degree d) allows the particle to have as many coin basis states. In irregular graphs, the degree is different for different

vertices, which causes the dimension of the coin Hilbert space to occupy a range of values, and hence, it becomes difficult to choose one coin to act on all the vertices. However, there are a couple of solutions one can employ. Self-loops can be used to effect regularity. Another solution is for the coin operator to depend on the vertex. Hence, $\hat{C}$ can be structured differently for different applications. In this paper we will consider only regular graphs.

The notion of vertex hitting time is a concept borrowed from classical random walks. Classically, it is defined as the average number of time steps taken for a walk to reach a “final” vertex v_f , given an initial distribution. The formula for the hitting time $\tau_h(v_f)$ is

$$\tau_h(v_f) = \sum_{t=0}^{\infty} t p(v_f, t), \quad (2)$$

where $p(v_f, t)$ is the probability that the walk has reached vertex v_f at time t for the first time.

Classical random walks will always have finite hitting times for all vertices in finite connected graphs. However, interference effects may prevent this in quantum walks. This leads to the uniquely quantum-mechanical phenomenon of an infinite hitting time.

To define a quantum notion of hitting time we must define what it means to arrive at a vertex for the first time. In our approach, we treat the final vertex as an absorbing wall. After every time step of the walk, a measurement is performed on the final vertex to check whether the walk has reached it or not. If it has, the walk is halted. The average time until the walk halts is the hitting time for the measured quantum walk.

The projective measurements used are $\hat{\Pi}_f = |v_f\rangle\langle v_f| \otimes \mathbf{1}_c$ and $\mathbf{1} - \hat{\Pi}_f$, where $|v_f\rangle$ is the state on the final vertex. For a detailed explanation, we refer the reader to Ref. [8].

Spectral analysis of the unitary evolution operator reveals that there may be some eigenvectors that have no overlap with the chosen final vertex v_f . If a component of the initial state $|\psi\rangle$ exists in the subspace spanned by these eigenvectors, that component never reaches the final vertex. This phenomenon may lead to infinite hitting time at the final vertex, so we label this the infinite-hitting-time (IHT) subspace, denoted as V . The overlap between the initial state and the IHT subspace quantifies the probability that the final vertex is never reached:

$$O_V(|\psi\rangle) = \sum_{i=1}^{|V|} |\langle \psi | V_i \rangle|^2, \quad (3)$$

where $\{V_i\}$ is an orthonormal basis for V .

A sufficient condition for infinite hitting times, established in [8–10], is for the evolution unitary to contain at least one k -dimensional eigenspace, where $k > d$. Within this eigenspace there will exist a subspace of dimension at least $k - d$ that has no support on the final vertex. This subspace forms a part of the IHT subspace. If multiple eigenspaces contain IHT subspaces, the sum of these subspaces gives the IHT subspace of the entire unitary.

While the above condition is sufficient for a quantum walk unitary to have an IHT subspace, it is not a necessary condition. It is possible for eigenspaces with degeneracy $\leq d$ to contain vectors that have no overlap with the final vertex. Hence, one must perform an analysis over all the eigenspaces when computing the size of the IHT subspace. The procedure is simple. Apply Gaussian elimination to each eigenspace, and subsequently count the number of vectors that have no overlap with a chosen final vertex.

In general, degenerate eigenspaces of the unitary contribute to the existence of IHT subspaces. This degeneracy is primarily a consequence of symmetry; hence, an analysis of the symmetries of the quantum walk may provide conditions predicting infinite hitting times.

II. SYMMETRIES OF A QUANTUM WALK

Previous work has focused on the influence of graph symmetry on infinite hitting time [9,10]. Here, the symmetry of the graph was represented by its group of direction-preserving automorphisms. The irreducible representations of this group give a sufficient condition for a quantum walk on this graph to have infinite hitting times. If the dimension of at least one of the irreducible representations is larger than the dimension of the coin, a corresponding eigenspace of the quantum walk unitary will have a larger dimension than the coin, which is a sufficient condition for a graph to exhibit infinite hitting times. These papers considered Cayley graphs, in which the automorphism group is simply related to the group used to define the graph. The first discovery of infinite hitting time [9] was observed on the n -dimensional hypercube with 2^n vertices, where $n \geq 3$.

An automorphism of a graph is a reordering of the vertices that leaves the graph unchanged. Since this reordering is just a permutation of the vertices, we can use permutation matrices

to define automorphisms. We consider two classes of permutations $\mathcal{P}_1 \subseteq \mathcal{P}_2 \subseteq \mathcal{P}$, where $\mathcal{P}$ is the set of all permutations on $\mathcal{H}$. $\mathcal{P}_1$ and $\mathcal{P}_2$ contain permutations with a tensor-product structure and are defined as

$$\mathcal{P}_1 = \{\hat{P} \mid \hat{P} = \hat{P}_v \otimes \mathbf{1}_c\} \quad (4)$$

and

$$\mathcal{P}_2 = \{\hat{P} \mid \hat{P} = \hat{P}_v \otimes \hat{P}_c\}, \quad (5)$$

where $\hat{P}_v$ and $\hat{P}_c$ are permutations acting on $\mathcal{H}_v$ and $\mathcal{H}_c$, respectively. Permutations $\hat{P}$ that give rise to graph automorphisms necessarily leave the shift operator invariant:

$$\mathcal{A} = \{\hat{P} \mid \hat{P}\hat{S}\hat{P}^\dagger = \hat{S}\}. \quad (6)$$

Thus, the group of *direction-preserving automorphisms* studied in [8–10] is generated from permutations in $\mathcal{P}_1$ that leave $\hat{S}$ invariant:

$$\mathcal{A}_1 = \{\hat{P} \in \mathcal{P}_1 \mid \hat{P}\hat{S}\hat{P}^\dagger = \hat{S}\}. \quad (7)$$

Here, we consider automorphisms from the larger class of permutations $\mathcal{P}_2$:

$$\mathcal{A}_2 = \{\hat{P} \in \mathcal{P}_2 \mid \hat{P}\hat{S}\hat{P}^\dagger = \hat{S}\}, \quad (8)$$

which forms the group of *joint automorphisms*. Clearly, $\mathcal{A}_1 \subseteq \mathcal{A}_2 \subseteq \mathcal{A}$.

Infinite hitting times in quantum walks are a consequence of symmetry in the quantum walk unitary $\hat{U}$. These symmetries can be represented by unitary operations $\hat{W}$ forming the group of quantum walk symmetries:

$$\mathcal{W} = \{\hat{W} \mid \hat{W}\hat{U}\hat{W}^\dagger = \hat{U}\}. \quad (9)$$

Hence, for a graph automorphism to be a symmetry of the quantum walk, it must satisfy $\hat{P}\hat{U}\hat{P}^\dagger = \hat{U}$. This is readily satisfied by all the elements of $\mathcal{A}_1$. Hence, the group of direction-preserving automorphisms actually contains symmetries of the quantum walk: $\mathcal{A}_1 = \mathcal{W}_1$. For elements in $\mathcal{A}_2$, the condition $\hat{P}\hat{U}\hat{P}^\dagger = \hat{U}$ is satisfied only when the coin permutation leaves the coin operator invariant:

$$\hat{P}_c\hat{C}\hat{P}_c^\dagger = \hat{C}. \quad (10)$$

The joint automorphisms that satisfy this condition are symmetries of the quantum walk and are denoted as the group of *coin-permutation symmetries*:

$$\mathcal{W}_2 = \{\hat{P} \in \mathcal{A}_2 \mid \hat{P}_c\hat{C}\hat{P}_c^\dagger = \hat{C}\}. \quad (11)$$

Evidently, coin symmetry plays a large role in determining the size of the group of coin-permutation symmetries. By choosing coins of varying symmetry, it may be possible to connect characteristics of the coin-permutation symmetry group to the existence of infinite hitting times.

Automorphisms of the graph from $\mathcal{W} \cap (\mathcal{A} \setminus \mathcal{A}_2)$ may still be symmetries of the quantum walk. We do not address symmetries of this type and leave it open to future research. Figure 1 summarizes the relations between the different symmetry groups discussed above.

III. COINS

In the analysis of infinite hitting times in quantum walks, we use three coins. On one end, we have the Grover coin,

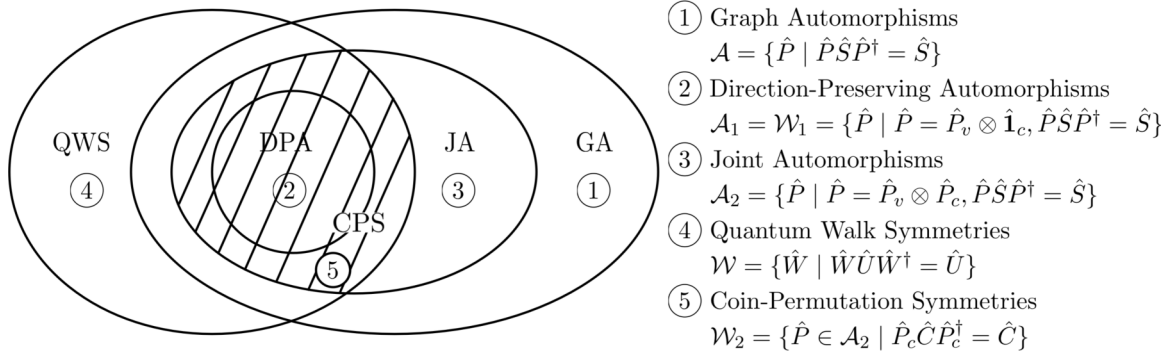


FIG. 1. Relations between classes of graph automorphisms and quantum walk symmetries.

which is the most symmetric of the lot. On the other end, we consider a random unitary, which should lack any particular symmetry. As an intermediate between these two, we also consider the discrete-Fourier-transform (DFT) coin.

Grover coin. This is the most symmetric coin generally used in quantum walks, and we would expect to see this symmetry reflected in the eigenspace decomposition of a walk's unitary. The symmetry arises from the permutation invariance [11] of the coin, which takes the form

$$\hat{G} = \begin{bmatrix} a & b & b & \cdots & b \\ b & a & b & \cdots & b \\ b & b & a & \cdots & b \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ b & b & b & \cdots & a \end{bmatrix}, \quad (12)$$

where we choose $a = \frac{2}{d} - 1$ and $b = \frac{2}{d}$ and d is the dimension of the coin. Due to the permutation-invariance property, all $d!$ permutation matrices $\hat{P}_c$ of size $d \times d$ satisfy the coin-permutation symmetry constraint: $\hat{P}_c\hat{G}\hat{P}_c = \hat{G}$, implying this coin is associated with the largest possible coin-permutation symmetry group.

The symmetries of this coin fit into the symmetries of the hypercube very nicely. A quantum walk on an n -dimensional hypercube with this coin can be reduced to a quantum walk on a line for the initial state $|0\rangle\langle 0| \otimes |\psi\rangle\langle\psi|$, where $|\psi\rangle = \frac{1}{\sqrt{n}} \sum_{j=1}^n |j\rangle$ [12].

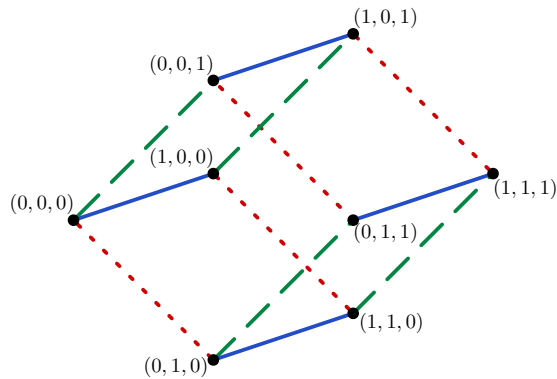


FIG. 2. The 3D cube, with solid blue, dashed green, and dotted red edges to signify logical XOR with 100, 001, and 010, respectively.

DFT coin. Another commonly used coin is the DFT coin $\hat{D}$. It is a generalization of the popular Hadamard coin $\hat{f}$ to arbitrary dimension:

$$\hat{f} = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad (13)$$

$$\hat{D} = \frac{1}{\sqrt{d}} \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 \\ 1 & \omega & \omega^2 & \cdots & \omega^{(d-1)} \\ 1 & \omega^2 & \omega^4 & \cdots & \omega^{2(d-1)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{(d-1)} & \omega^{(d-1)2} & \cdots & \omega^{(d-1)(d-1)} \end{bmatrix}, \quad (14)$$

where $\omega = e^{i2\pi/d}$. This coin is not as symmetric as the Grover coin, and we see this reflected in our analysis of quantum walk unitaries. For a DFT coin of any dimension, there are only two permutation matrices that leave the coin invariant. The identity permutation gives rise to direction-preserving automorphisms; however, the permutation $(1, d, d-1, \dots, 3, 2)$ can create joint automorphisms. The associated coin-permutation symmetry group is hence smaller than that for the Grover coin; however, $\mathcal{W}_1 \subsetneq \mathcal{W}_2$.

Asymmetric coin. Our last coin is a random unitary. To create this unitary, we generate a matrix of random complex numbers and subsequently orthogonalize it. Here we expect $\mathcal{W}_1 = \mathcal{W}_2$.

TABLE I. Spectral decomposition of the unitary $\hat{U}$ for walks on the 3D cube. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 24$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k| = \sum m_k |V_k|$.

Coin	Eigenspaces				IHT?
	k	m_k	$ V_k $	$ V $	
Grover	6	2	3	6	Yes
	3	4	0		
DFT	2	2	1	2	Yes
	2	8	0		
	1	4	0		
Asymmetric	1	24	0	0	No

TABLE II. Spectral decomposition of the unitary $\hat{U}$ for walks on the four-dimensional (4D) hypercube. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 64$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k|$.

Coin	Eigenspaces			$ V $	IHT?
	k	m_k	$ V_k $		
Grover	18	2	14	32	Yes
	6	2	2		
	4	4	0		
DFT	8	4	5	24	Yes
	4	4	1		
	2	8	0		
Asymmetric	1	64	0	0	No

IV. SPECTRAL ANALYSIS OF QUANTUM WALK UNITARIES

Using the coins from the previous section, we constructed quantum walk unitaries for multiple Cayley graphs. We consider Cayley graphs since their construction always yields d -regular graphs, and their automorphism groups are closely related to the groups used to construct them. In particular we look at Cayley graphs of the Abelian $\mathbb{Z}_2^d$ group (hypercube of dimension d) and symmetric groups of different sizes.

Cayley graphs are defined using a group G and a generating set $H \subseteq G$. The elements $g_i \in G$ form the vertices of the Cayley graph, and edges exist between two vertices g_i and g_j if $g_i g_j^{-1} \in H$. In other words, an element of H , say, h_j , defines an edge between g_i and g_j when $h_j g_i = g_j$. Thus, each element of G will have $|H|$ edges, making it an $|H|$ -regular graph. H is called a generating set if and only if its elements produce a Cayley graph that is connected.

The shift operator $\hat{S}$ for Cayley graphs will thus be

$$\hat{S} = \sum_{i=0}^{|G|-1} \sum_{j=0}^{|H|-1} |h_j g_i, j\rangle \langle g_i, j|, \quad (15)$$

TABLE III. Spectral decomposition of the unitary $\hat{U}$ for walks on the 5D hypercube. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 160$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k|$.

Coin	Eigenspaces			$ V $	IHT?
	k	m_k	$ V_k $		
Grover	50	2	45	110	Yes
	10	4	5		
	5	4	0		
DFT	10	2	7	22	Yes
	4	2	2		
	2	4	1		
	2	60	0		
	1	4	0		
Asymmetric	1	160	0	0	No

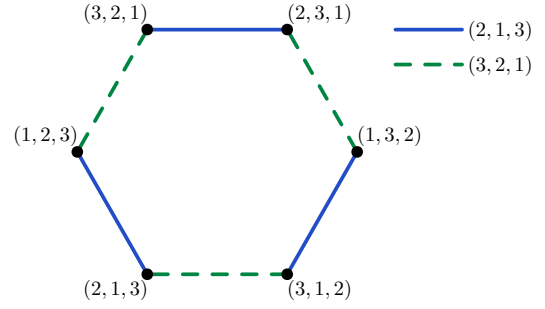


FIG. 3. The Cayley graph of S_3 with generating set $H = \{(2,1,3), (3,2,1)\}$, where application of the permutation $(2,1,3)$ corresponds to a blue solid edge and $(3,2,1)$ corresponds to a green dashed edge.

where $h_j g_i$ is the group composition operation between two elements h_j and g_i .

A. Hypercubes: Cayley graphs of Abelian group $\mathbb{Z}_2^d$

In a hypercube, vertices can be labeled using bit strings from $\mathbb{Z}_2^d$. Hence, a d -dimensional hypercube has a vertex Hilbert space $\mathcal{H}_v$ of size 2^d . Two vertices labeled by bit strings x and y are connected if x and y differ in exactly one bit, that is,

$$h(x \oplus y) = 1,$$

where $h(a)$ is the Hamming weight of string a and $x \oplus y$ is the bitwise XOR of the bit strings corresponding to vertices x and y . In the Cayley graph formalism, this implies the generating set H contains all weight-one bit strings. For any vertex x , there can be only d other bit strings which satisfy the above equation; hence, each vertex of the hypercube has degree d . Thus, each vertex has d basis states, and the dimension of the coin Hilbert space $\mathcal{H}_c$ is also d . Thus, the unitary describing the evolution of states in a hypercube will be of dimension $|\mathcal{H}_c| |\mathcal{H}_v| = d 2^d$. The three-dimensional (3D) cube is displayed as an example in Fig. 2.

The hypercube is an interesting case because it does not satisfy the sufficient condition derived in [9] for a graph to exhibit quantum walks with infinite hitting times. Its automorphism group is Abelian, and all its irreducible representations have dimension 1. However, it was observed in [9] that walks

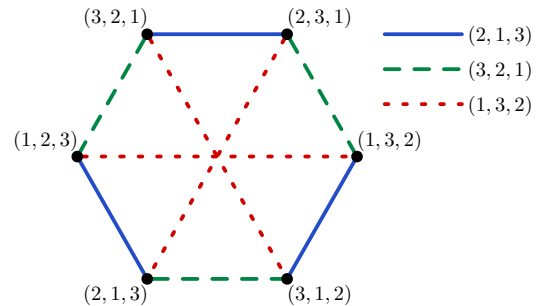


FIG. 4. The Cayley graph of S_3 with generating set $H = \{(2,1,3), (3,2,1), (1,3,2)\}$, where application of the permutation $(2,1,3)$ corresponds to a blue solid edge, $(3,2,1)$ corresponds to a green dashed edge, and $(1,3,2)$ corresponds to a red dotted edge.

TABLE IV. Spectral decomposition of the unitary $\hat{U}$ for walks on the Cayley graph of S_3 with generating set $H = \{(2, 1, 3), (3, 2, 1), (1, 3, 2)\}$. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 18$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k|$.

Coin	Eigenspaces			$ V $	IHT?
	k	m_k	$ V_k $		
Grover	5	2	2	6	Yes
	4	2	1		
DFT	4	2	1	2	Yes
	2	4	0		
	1	2	0		
Asymmetric	2	6	0	0	No
	1	6	0		

on the hypercube can, indeed, exhibit infinite hitting times with some coins. This was presumed to be an effect of the coin symmetry. In this paper, we can now validate that intuition.

In the hypercube, the shift operator $\hat{S}$ can be expressed as

$$\hat{S} = \sum_{x=0}^{2^d-1} \sum_{j=0}^{d-1} |x \oplus e_j\rangle \langle x, j|, \quad (16)$$

where e_j is the n -bit string corresponding to the number 2^j and the notation $|a, b\rangle \equiv |a\rangle \otimes |b\rangle$. Thus, the shift operator transfers the state from vertex x along edge j to the vertex $x \oplus e_j$.

We analyzed the evolution unitary for hypercubes of dimensions 3, 4, and 5. We choose the vertex labeled $2^d - 1$ to be the final vertex with the absorbing wall. Thus, the projector onto the final vertex is $\hat{\Pi}_f = |2^d - 1\rangle \langle 2^d - 1| \otimes \hat{\mathbf{1}}_d$. To avoid infinite hitting time at this final vertex, one must ensure that the initial state has no components in the IHT subspace of the unitary. Note that the IHT subspace depends only on the choice of the final vertex.

The results of spectral decomposition of the unitaries are displayed in Tables I, II, and III. For each of the proposed quantum walks in this paper, we ask whether the walk may potentially exhibit infinite hitting time or not. The lack of graph symmetry is highlighted by the fact that there are no degenerate eigenspaces in any of the unitaries using the asymmetric coin.

First, we note that infinite hitting times are possible in all the tested hypercubes for quantum walks that use the Grover or DFT coin. As illustrated in Tables I–III, the dimension of the IHT subspace is generally larger for quantum walks

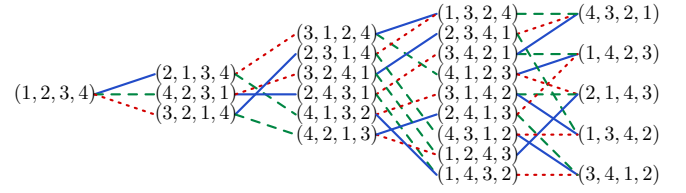


FIG. 6. The Cayley graph of S_4 with generating set $H_2 = \{(2, 1, 3, 4), (3, 2, 1, 4), (4, 2, 3, 1)\}$, where application of the permutation $(2,1,3,4)$ corresponds to a blue solid edge, $(4,2,3,1)$ corresponds to a green dashed edge, and $(3,2,1,4)$ corresponds to a red dotted edge.

that use the Grover coin than those that use the DFT coin. For larger hypercubes, the ratio of the dimension of the IHT subspace to the dimension of the Hilbert space grows asymptotically to 1 (for $d = 9$, $|\mathcal{H}| = 4608$, $|V|/|\mathcal{H}| = 0.965$).

For quantum walks that use the DFT coin, eigenspaces of dimension $< d$ also contain vectors in the IHT subspace. This is interesting as these eigenspaces do not satisfy the previously shown sufficient condition for the existence of IHT subspaces, that the dimension of at least one eigenspace is larger than that of the coin. We additionally observed that the ratio of the dimension of the IHT subspace to the dimension of the Hilbert space $|V|/|\mathcal{H}|$ is generally larger for the DFT coin in even dimensions as opposed to odd dimensions. We were able to observe this effect up to coin dimension 11, as performing the decomposition for larger dimensions becomes computationally expensive. Further work is needed to understand the systematic differences between even and odd dimensions.

B. Cayley graphs of the symmetric group

We consider Cayley graphs of symmetric groups with different generating sets. For groups S_3 and S_4 we consider elements $(1,2,3)$ and $(1,2,3,4)$, respectively, as the final vertices.

S_3 with generating set $H = \{(2, 1, 3), (3, 2, 1)\}$. This Cayley graph is a circle of the six elements of S_3 , as shown in Fig. 3. Quantum walks on the circle do not exhibit infinite hitting time except when the coin operator is the identity.

S_3 with generating set $H = \{(2, 1, 3), (3, 2, 1), (1, 3, 2)\}$. When we add the permutation element $(1,3,2)$ to the generating set, the graph becomes more connected. As shown in Fig. 4, every vertex is now within two edges of every other vertex. However, quantum walks on this graph can still exhibit infinite hitting times with the Grover and DFT coins. Decomposition of the evolution unitary yields eigenspaces as in Table IV. For the Grover coin, each of the individual subspaces has greater than three dimensions. So they each

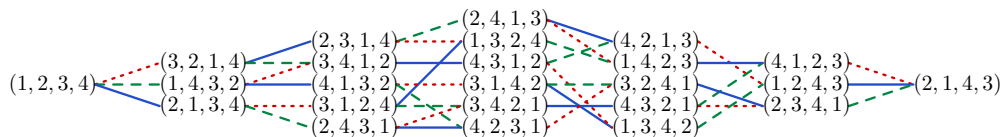


FIG. 5. The Cayley graph of S_4 with generating set $H_1 = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 4, 3, 2)\}$, where application of the permutation $(2,1,3,4)$ corresponds to a blue solid edge, $(1,4,3,2)$ corresponds to a green dashed edge, and $(3,2,1,4)$ corresponds to a red dotted edge.

TABLE V. Spectral decomposition of the unitary $\hat{U}$ for walks on the Cayley graph of S_4 with generating set $H_1 = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 4, 3, 2)\}$. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 72$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k|$.

Coin	Eigenspaces			$ V $	IHT?
	k	m_k	$ V_k $		
Grover	14	2	11	26	Yes
	3	4	1		
	3	8	0		
	2	4	0		
DFT	6	2	5	15	Yes
	3	5	1		
	3	11	0		
	2	6	0		
Asymmetric	3	18	0	0	No
	2	6	0		
	1	6	0		

include subspaces that have no overlap with the final vertex. The size of the IHT subspace with the Grover coin is six. For the DFT coin, we observe a smaller IHT subspace, of dimension 2. Although quantum walks with the asymmetric coin do not actually exhibit infinite hitting times, there are degenerate eigenspaces in the evolution unitary. This degeneracy arises from the symmetry of the graph, as explored in Refs. [9,10].

S_4 with generating sets $H_1 = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 4, 3, 2)\}$, $H_2 = \{(2, 1, 3, 4), (3, 2, 1, 4), (4, 2, 3, 1)\}$. When looking at Cayley graphs of S_4 , we can observe the combined effect of coin symmetry and graph symmetry. We consider two generating sets of the same size to understand how graph symmetry plays a role in producing larger IHT

TABLE VI. Spectral decomposition of the unitary $\hat{U}$ for walks on the Cayley graph of S_4 with generating set $H_2 = \{(2, 1, 3, 4), (3, 2, 1, 4), (4, 2, 3, 1)\}$. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 72$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k|$.

Coin	Eigenspaces			$ V $	IHT?
	k	m_k	$ V_k $		
Grover	14	2	11	36	Yes
	6	4	3		
	4	2	1		
	3	4	0		
DFT	4	2	3	14	Yes
	4	2	1		
	3	6	1		
	3	10	0		
Asymmetric	2	4	0	0	No
	3	18	0		
	1	6	0		

TABLE VII. Spectral decomposition of the unitary $\hat{U}$ for walks on the Cayley graph of S_4 with generating set $H = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 2, 4, 3), (1, 3, 2, 4)\}$. There exist m_k eigenspaces of dimension k , each with corresponding IHT subspace V_k of dimension $|V_k| < k$. The Hilbert space dimension is $|\mathcal{H}| = \sum m_k k = 96$, and the total IHT subspace dimension is $|V| = \sum m_k |V_k|$.

Coin	Eigenspaces			$ V $	IHT?
	k	m_k	$ V_k $		
Grover	26	2	22	56	Yes
	6	2	2		
	5	4	2		
	3	4	0		
DFT	11	2	8	35	Yes
	6	2	4		
	6	2	2		
	3	7	1		
Asymmetric	2	7	0	0	No
	2	4	0		
	3	24	0		
	2	8	0		
	1	8	0		

subspaces. Although H_1 and H_2 contain similar elements, they produce different Cayley graphs. H_1 generates a Cayley graph which can have a maximum separation of up to six edges between two elements, as shown in Fig. 5, whereas H_2 generates a Cayley graph that requires no more than four edges to reach every other vertex. The Cayley graph corresponding to this generating set is displayed in Fig. 6. Both graphs exhibit infinite hitting times, as shown in Tables V and VI. The most symmetric case, with generating set H_2 and the Grover coin, yields the IHT subspace with the largest dimension, 36:

Generating set	Grover	DFT
$H_1 = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 4, 3, 2)\}$	26	15
$H_2 = \{(2, 1, 3, 4), (3, 2, 1, 4), (4, 2, 3, 1)\}$	36	14

Curiously, the dimensions of the IHT subspaces for unitaries with the DFT coin are roughly the same, although one graph is more symmetric than the other. Using the asymmetric coin, the unitary has eigenspaces of degeneracy 3, which arise due to symmetries of the shift matrix $\hat{S}$. However, this degeneracy is insufficient to produce IHT subspaces.

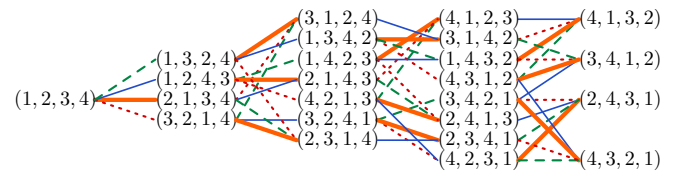


FIG. 7. The Cayley graph of S_4 with generating set $H = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 2, 4, 3), (1, 3, 2, 4)\}$, where application of the group element $(2,1,3,4)$ corresponds to a thick orange solid edge, $(3,2,1,4)$ corresponds to a red dotted edge, $(1,2,4,3)$ corresponds to a thin blue solid edge, and $(1,3,2,4)$ corresponds to a green dashed edge.

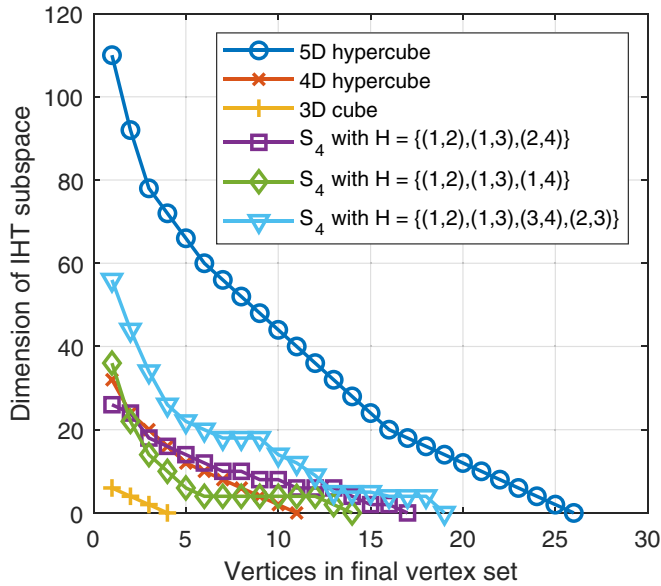


FIG. 8. Reduction in the dimension of the IHT subspace as the number of vertices in the final vertex set is increased. The evolution unitaries of six graphs with the Grover coin were analyzed.

S_4 with generating set $H = \{(2, 1, 3, 4), (3, 2, 1, 4), (1, 2, 4, 3), (1, 3, 2, 4)\}$. With a larger generating set, this graph has greater symmetry than the previous examples. This set generates a graph where the maximum separation between two vertices is four edges, as displayed in Fig. 7. Table VII presents the dimensions of the IHT subspaces of the evolution unitary for the different coins. The dimensions of the IHT subspaces with the Grover and DFT coins are 56 and 35, respectively. As expected, the increased graph symmetry enlarges the dimension of the IHT subspace in proportion to the Hilbert space. Spectral analyses of other Cayley graphs of S_4 with generating sets of size 4 also yield IHT subspaces which are larger than with three generating elements.

C. Multiple-vertex infinite hitting time

Until now hitting times have been calculated for only one final vertex. However, similar analyses can be made by considering a subset of the vertices to be “final” vertices. Increasing the number of final vertices leads to IHT subspaces of smaller dimension, and the corresponding overlap between the initial state and the IHT subspace decreases. This is illustrated in Fig. 8, which displays the dimension of the IHT

subspace for walks using the Grover coin on graphs with different numbers of final vertices. It is interesting to note that infinite hitting times are possible in the five-dimensional (5D) hypercube even if up to 25 of the 32 vertices are in the final vertex set. Similarly, for the Cayley graph of S_4 with four generating elements, there exists a nontrivial IHT subspace even if up to 18 of the 24 vertices are in the final vertex set.

V. CONCLUSION

The objective of this paper was to explore the influence of coin symmetry on infinite hitting time. We did not find an exact relationship between the group of coin-permutation symmetries and the dimension of the IHT subspace. However, we showed through analysis of three coins—the Grover coin, invariant under any permutation matrix; the DFT coin, invariant under only two permutation matrices; and random unitary coins lacking any symmetry—that coins with high symmetry and hence larger coin-permutation symmetry groups are associated with larger IHT subspaces. The dimensions of the IHT subspaces for some quantum walks that use these coins are summarized in Table VIII. Larger IHT subspaces generally imply a larger overlap with initial states, leading to a higher probability of never reaching the final vertex.

We also explored the effect of considering a group of vertices as final vertices, a final vertex set. It is interesting to note that these quantum walks can still exhibit infinite hitting time, as in the case of the 5D hypercube, which exhibits infinite hitting time with as many as 25 vertices in the final vertex set. Analyses of this type could be useful to determine beforehand the propensity of initial states to hit a set of target vertices in a graph. Conversely, this can also be used to choose graphs and coins to block initial states from reaching a set of target vertices.

A number of open questions remain about infinite hitting times in quantum walks. Is it possible to determine a sufficient condition for infinite hitting times using the irreducible representations of the coin-permutation symmetry group? Can we use analyses of infinite hitting times to solve or simplify computational problems? Are there larger automorphism groups or different types of quantum walk symmetries that more fully characterize infinite hitting times in quantum walks?

ACKNOWLEDGMENTS

P.P. and T.A.B. would like to acknowledge helpful conversations with N. Anand, C. Cantwell, Y.-H. Chen, C. Sutherland, and P. Zanardi. This work was supported in part by NSF Grants No. QIS-1719778 and No. FET-1911089.

TABLE VIII. Summary of results. The dimension of the IHT subspace $|V|$ for one final vertex is shown relative to the dimension of the unitary’s Hilbert space $|\mathcal{H}|$. Quantum walks with initial states having components in V can exhibit infinite hitting time on the chosen final vertex. $S_{i,j}$ is shorthand for a Cayley graph of the symmetric group S_i with a generating set of size j .

	3D cube	4D hypercube	5D hypercube	$S_{3,2}$	$S_{3,3}$	$S_{4,3}$	$S_{4,3}$	$S_{4,4}$
$ V $ for Grover coin	6	32	110	0	6	26	36	56
$ V $ for DFT coin	2	24	22	0	2	15	14	35
$ V $ for asymmetric coin	0	0	0	0	0	0	0	0
$ \mathcal{H} $	24	64	160	12	18	72	72	96

- [1] K. Pearson, The problem of the random walk, *Nature (London)* **72**, 294 (1905).
- [2] S. E. Venegas-Andraca, Quantum walks: A comprehensive review, *Quantum Inf. Process.* **11**, 1015 (2012).
- [3] J. Kempe, Quantum random walks: An introductory overview, *Contemp. Phys.* **50**, 339 (2009).
- [4] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, One-dimensional quantum walks, in *Proceedings of the Thirty-Third Annual ACM Symposium on Theory of Computing (STOC'01)* (ACM, New York, 2001), p. 37.
- [5] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, Quantum walks on graphs, in *Proceedings of the Thirty-Third Annual ACM Symposium on Theory of Computing (STOC'01)* (ACM, New York, 2001), p. 50.
- [6] E. Farhi and S. Gutmann, Quantum computation and decision trees, *Phys. Rev. A* **58**, 915 (1998).
- [7] A. M. Childs, E. Farhi, and S. Gutmann, An example of the difference between quantum and classical random walks, *Quantum Inf. Process.* **1**, 35 (2002).
- [8] H. Krovi and T. A. Brun, Quantum walks on quotient graphs, *Phys. Rev. A* **75**, 062332 (2007).
- [9] H. Krovi and T. A. Brun, Hitting time for quantum walks on the hypercube, *Phys. Rev. A* **73**, 032341 (2006).
- [10] H. Krovi and T. A. Brun, Quantum walks with infinite hitting times, *Phys. Rev. A* **74**, 042334 (2006).
- [11] C. Moore and A. Russell, Quantum walks on the hypercube, in *Proceedings of the 6th International Workshop on Randomization and Approximation Techniques in Computer Science (RANDOM 2002)*, edited by J. D. P. Rolim and S. Vadhan (Springer, Berlin, 2002), p. 164.
- [12] N. Shenvi, J. Kempe, and K. B. Whaley, Quantum random-walk search algorithm, *Phys. Rev. A* **67**, 052307 (2003).