2021-10-29

Quantum Walks on Arc-Transitive Graphs with Self-Loops

Yu, Zhan

UNIVERSITY OF CALGARY

Quantum Walks on Arc-Transitive Graphs with Self-Loops

by

Zhan Yu

A THESIS

SUBMITTED TO THE FACULTY OF GRADUATE STUDIES

IN PARTIAL FULFILLMENT OF THE REQUIREMENTS FOR THE

DEGREE OF MASTER OF SCIENCE

GRADUATE PROGRAM IN COMPUTER SCIENCE

CALGARY, ALBERTA

OCTOBER, 2021

Abstract

The lackadaisical quantum walk is a quantum analogue of the lazy random walk obtained by adding a self-loop to each vertex in the graph. The lackadaisical quantum walk has been studied on cycles, n-dimensional tori, hypercubes, Johnson graphs, and other classes of vertex-transitive graphs. The results of numerical simulation show that lackadaisical quantum walks can find a unique marked vertex on these graphs with constant success probability quadratically faster than the random walk, and the optimal weight of the self-loops is $\ell = \frac{d}{N}$ where d is the degree of the vertices and N is the number of vertices. One common property of these classes of graphs is that they are locally arc-transitive.

In this thesis, we analytically prove that for any d-regular locally arc-transitive graph, by adding a self-loop of weight $\ell = \frac{d}{N}$ on each vertex, the lackadaisical quantum walk finds a unique marked vertex with probability at least a constant. Our proof establishes and uses a relationship between the lackadaisical quantum walk and the quantum interpolated walk that was introduced by Krovi, Magniez, Ozols, and Roland in 2015. Our result proves speculations and numerical findings of lackadaisical quantum walks in previous work.

Preface

The result presented in this thesis has been published as Peter Høyer and Zhan Yu, "Analysis of Lackadaisical Quantum Walks", Quantum Information and Computation, Vol. 20, No. 13–14 (2020) 1137–1152, by Rinton Press. The contents of this article are used in Chapter 5 of this thesis either verbatim or with some modifications as required.

Acknowledgements

First I would like to express my deepest appreciation to my supervisor Dr. Peter Høyer. He consistently supported and encouraged me even when the road got tough. I am grateful for his guidance, both in academic and non-academic matters, to ensure that I always left Jabberwocky infused with inspiration and enthusiasm.

I am also grateful to my committee members Dr. Robin Cockett and Dr. Renate Scheidler for serving as examiners along with Peter. Many thanks to them for taking the time to read my thesis and provide insightful comments.

During my undergraduate and graduate studies in University of Calgary, I have been fortunate to be a part of a fantastic research group. I would like to thank current and former members of our group, Dante Bencivenga, Xining Chen, Cătălin Dohotaru, Elliot Evans, Janet Leahy, Shang Li, Alireza Poostindouz, Arta Seify, Yehonatan Shabash, and Spencer Wilson. I am grateful to them for their inspiring discussions with me, their help on my study and research, and all the joy they brought me. I have benefited greatly from the environment of intellectual creativity and curiosity in the group. Special thanks to Dante Bencivenga, Xining Chen, and Janet Leahy, who helped in editing and revising this thesis. Their useful feedback is appreciated.

Lastly, my deep and sincere gratitude to my family and friends for their continuous support. I especially thank my parents for their unconditional love, patience and belief they have shown me throughout my entire life.

To all the time I've wasted...

Table of Contents

List of Figures and Illustrations

Chapter 1

Introduction

Searching is one of the most important tasks in computer science. Searching structured databases can be modelled as spatial search problems on graphs. A subset of the vertices are marked, and the goal is to find one of the marked vertices. Searching algorithms have been well studied from both classical and quantum aspects. One classical strategy is to use a random walk to traverse the graph along its edges until a marked vertex is reached. The expected number of steps required to reach a marked vertex by a random walk is called the hitting time and denoted as HT.

Quantum walks, which are quantum counterparts of random walks, are used to develop quantum algorithms for spatial search problems. Szegedy introduced a general method of constructing a quantum walk from a reversible random walk [Sze04]. The resulting quantum walk uses $O(\sqrt{\mathsf{HT}})$ steps, which yields a quadratic speedup over the random walk. Szegedy's algorithm does not necessarily find a marked vertex, but it can detect the presence of a marked vertex. Krovi et al. [KMOR16] later proposed a quantum algorithm based on the novel idea of interpolated walks. They applied Szegedy's correspondence on the interpolated walks and called the resulting algorithms quantum interpolated walks. Quantum interpolated walks can find a unique marked vertex in $O(\sqrt{\mathsf{HT}})$ steps for any reversible random walk. Dohotaru and Høyer [DH17] achieved the same result by introducing a different framework called controlled quantum walks.

Quantum walks are commonly applied on graphs without self-loops. The lackadaisical quantum walk proposed by Wong [Won15], is a quantum analogue of the lazy random walk, which adds a self-loop of weight ℓ to each vertex of the graph. The lackadaisical quantum walk has been studied on several classes of graphs including complete graphs [AKR05, Won15, Won18a, Won17], n-dimensional tori [WZWY17, Won18b, GK20], and regular bipartite graphs [RW19]. The results show that adding a self-loop on each vertex increases the success probability of finding a marked vertex, compared to the loopless quantum walk. Rhodes and Wong [RW20] observe that these graphs are all vertex-transitive, and they study a collection of vertex-transitive graphs. They numerically show that by setting $\ell = \frac{d}{N}$, the lackadaisical quantum walk finds a unique marked vertex with probability at least a constant. Here d is the degree of the vertices. They propose that this holds for all vertex-transitive graphs with a unique marked vertex, and the weight of self-loop $\ell = \frac{d}{N}$ is optimal. The result is strongly supported by the experiments and stated as a conjecture.

In this thesis, we analytically prove the complexity and success probability of lackadaisical quantum walks on graphs as listed above. More generally, we prove that for any d-regular locally arc-transitive graph, by adding a self-loop of weight $\ell = \frac{d}{N}$ on each vertex, the lackadaisical quantum walk finds a unique marked vertex with probability at least a constant in $O(\sqrt{\mathsf{HT}})$ steps. In our proof, we establish and use relationships between lackadaisical quantum walks and quantum interpolated walks for any regular locally arc-transitive graph with a unique marked vertex. This relationship provides a new perspective to analyze these two quantum walks.

1.1 Outline

In this chapter, we introduce basic concepts involved in quantum computations, graphs, and random walks. In Chapter 2, we present Szegedy's correspondence to construct a quantum walk, which solves the detecting problem quadratically faster than a random walk. In Chapter 3, we introduce quantum interpolated walks then prove the complexity and success probability of quantum interpolated walks to solve search problems. In Chapter 4, we introduce the lackadaisical quantum walk and present known results in previous work.

Our original contribution is in Chapter 5, where we prove the complexity and success probability of lackadaisical quantum walks on locally arc-transitive graphs with a unique marked vertex. Our main results are stated as Theorem 29 and Theorem 35. Theorem 29 states that the quantum hitting time of lackadaisical quantum walks and quantum interpolated walks are of the same order. Theorem 35 states that the L^2-distance between the two quantum states of the lackadaisical quantum walk and the quantum interpolated walk, respectively, remains negligible for any number of steps that is in the order of the quantum hitting time. The two theorems hold for any regular locally arc-transitive graph with a unique marked vertex. By combining the two main Theorems with the analysis of quantum interpolated walks in Chapter 3, we complete the analytical proofs of the complexity and success probability of lackadaisical walks on regular locally arc-transitive graphs.

The main technical contribution in our work is the use of local arc-transitivity to establish a connection between lackadaisical quantum walks and quantum interpolated walks. The definition of local arc-transitivity is given in Section 1.3.2. We discuss the relationship between local arc-transitivity, vertex-transitivity and other graph properties in Appendix A.

1.2 Quantum Computation

In this section, we introduce basic concepts of quantum computation. One can refer to [NC00] for more details.

1.2.1 Quantum states

The *bit* is the basic unit of information in classical computation. Quantum computation and quantum information use an analogous concept, the *quantum bit*, or *qubit* for short. Just as a classical bit has a *state* in either 0 or 1, a qubit also has a state. The state of a qubit is a unit vector in a 2-dimensional Hilbert space $\mathcal{H}_2 = \mathbb{C}^2$. Two possible states for a qubit are the states $|0\rangle$ and $|1\rangle$, which are known as computational basis states. The notation "$|\rangle$" is called a *ket*, which represents a column vector in a Hilbert space. The conjugate transpose of a ket, which is a row vector in a Hilbert space, is called a *bra*. We denote a bra by the notation "$\langle|$". This notation is called *bra-ket notation*, or *Dirac notation*. In quantum computing, a *quantum register* is a system comprising multiple qubits, which is the quantum analogue of the classical processor register.

The difference between bits and qubits is that a qubit can be in linear combinations of states, also called *superpositions*,

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle,$$

where $\alpha, \beta \in \mathbb{C}$ are *amplitudes* of states $|0\rangle$ and $|1\rangle$, respectively. Note that $|\psi\rangle$ is a normalized state so $|\alpha|^2 + |\beta|^2 = 1$. More generally, we can use a normalized vector $|\Psi\rangle$ in the N-dimensional Hilbert space $\mathcal{H}_N = \mathbb{C}^{2^n}$ to represent a quantum state of an n-qubit quantum computer:

$$|\Psi\rangle = \sum_{k=0}^{N-1} \alpha_k |k\rangle, \tag{1.1}$$

where $\{|k\rangle : k = 0, \ldots, N-1\}$ forms an orthonormal basis of $\mathcal{H}_N$ and $\sum_{k=0}^{N-1} |\alpha_k|^2 = 1$.

Given two quantum states $|\psi\rangle \in \mathcal{H}_A$ and $|\phi\rangle \in \mathcal{H}_B$, the combined state of $|\psi\rangle$ and $|\phi\rangle$ is a tensor product $|\psi\rangle \otimes |\phi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$. In this thesis, we often omit the symbol $\otimes$ and write the tensor prodcut state as $|\psi\rangle|\phi\rangle$, or simply $|\psi, \phi\rangle$.

1.2.2 Quantum measurements

Measuring the state $|\Psi\rangle$ from Equation 1.1 with respect to the orthonormal basis $\{|k\rangle : k = 0, \ldots, N-1\}$ produces the basis state $|k\rangle$ with probability $|\langle\Psi|k\rangle|^2 = |\alpha_k|^2$. Such a measurement is called a *basis measurement*. After the basis measurement, the state $|\Psi\rangle$ collapses to a basis state $|k\rangle$.

More generally, we can divide the Hilbert space $\mathcal{H}_N$ into multiple orthogonal subspaces $\{\mathcal{H}_{N,j}\}$. Let $\Pi_j = \sum_k |b_{j,k}\rangle\langle b_{j,k}|$ be a projection onto the subspace $\mathcal{H}_{N,j}$ where $\{|b_{j,k}\rangle\}_k$ is the orthonormal basis of $\mathcal{H}_{N,j}$. Then the collection of mutually orthogonal projections $\{\Pi_j\}$ is a *projective measurement* on the Hilbert space $\mathcal{H}_N$.

Upon measuring the state $|\psi\rangle$, the probability of getting a result in the subspace $\mathcal{H}_{N,j}$ is $\langle\psi|\Pi_j|\psi\rangle$, and the state immediately after the measurement is

$$\frac{\Pi_j|\psi\rangle}{\sqrt{\langle\psi|\Pi_j|\psi\rangle}}.$$

Note that the basis measurement is a special case of projective measurement, where we divide the Hilbert space $\mathcal{H}_N$ into N orthogonal subspaces.

1.2.3 Quantum operators

Other than measuring a state, we can also apply some operations to change the state. A postulate of quantum computing is that quantum evolution other than measurements is *unitary*. That is, if we have a quantum operator W that takes an input state $|\psi\rangle$ and outputs a state $\mathsf{W}|\psi\rangle$, then we can describe W as a *unitary linear transformation*. In this thesis, other than quantum measurements, we only consider unitary quantum operators.

An operator W is unitary if it satisfies $\mathsf{W}^\dagger\mathsf{W} = \mathsf{W}\mathsf{W}^\dagger = \mathsf{I}$, where $\mathsf{W}^\dagger$ is the adjoint of W. A unitary operator W has the following properties:

- The rows of the operator W form an orthonormal basis.
- The columns of the operator W form an orthonormal basis.
- The operator W preserves inner products, i.e. $\langle\psi|\mathsf{W}^\dagger\mathsf{W}|\phi\rangle = \langle\psi|\phi\rangle$. Therefore, W preserves L^2-norms.
- The spectral decomposition of W is

  $$\mathsf{W} = \sum_j e^{i\theta_j}|v_j\rangle\langle v_j|,$$

  where $\{|v_j\rangle\}_j$ are orthonormal eigenvectors of W corresponding to eigenvalues $\{e^{i\theta_j}\}_j$.

We can represent quantum operators using circuit diagrams. Figure 1.1 shows a circuit representing the application of a quantum operator W to a quantum state $|\psi\rangle$. We use rectangular boxes to represent quantum operators. Note that the quantum operators are applied to quantum states from the left, but quantum circuits are applied left-to-right, i.e. quantum states are input from the left of the circuit and output on the right-hand side.

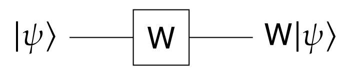

Figure 1.1: Circuit representing the application of a quantum operator W to a state $|\psi\rangle$.

Other than the directly-applied quantum operators, there is another class of operators in quantum computing called controlled operators, which is shown in Figure 1.2. We use a circle to represent a control. In Figure 1.2, the upper register is for control and the lower one is the operation register. The controlled operator c-W applies the quantum operator W on the operation register if the control register is in the state $|c\rangle$, otherwise it applies an identity to the operation register. We can write the controlled operator c-W in the form of $|c\rangle\langle c| \otimes \mathsf{W} + (\mathsf{I} - |c\rangle\langle c|) \otimes \mathsf{I}$.

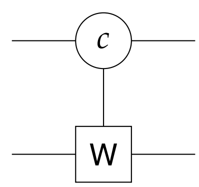

Figure 1.2: Circuit of a controlled operator c-W.

1.3 Graphs

An *undirected graph* is a pair $G = (V, E)$, where V is a set of *vertices*, and E is a set of *undirected edges*, which are unordered multisets of two vertices. The edges of a graph define the *adjacency relation* on the vertices. Two vertices x and y are adjacent if $\{x, y\}$ is an edge.

A *directed graph* is a pair $G = (V, D)$, where V is a set of vertices, and D is a set of *directed edges*, often called *arcs*. An arc is an ordered pair of adjacent vertices. In this thesis, we will interchangeably consider an undirected graph as a directed graph, where we consider each edge $\{x, y\}$ between two distinct vertices as two arcs (x, y) and (y, x).

A *self-loop* is an edge $\{x, x\}$ or an arc (x, x) that connects the vertex x to itself. When we consider an undirected graph as a directed graph, each edge $\{x, x\}$ is considered as one arc (x, x).

A *simple graph* is an unweighted, undirected graph containing no self-loops and no multi-edges between two vertices. Using the adjacency relation, a simple graph containing N vertices can be fully specified by its *adjacency matrix* A, which is an $N \times N$ matrix. Each entry $A_{xy} \in \{1, 0\}$ indicates that x and y are adjacent or nonadjacent, respectively.

In graph theory, the *degree* of a vertex x is the number of edges that are incident to x, denoted by $\deg(x)$. A graph is *d-regular* if each vertex has degree d.

1.3.1 Self-loops

In this thesis, we always start with simple graphs, and we may modify them by adding weighted self-loops. In other words, we consider graphs where all edges except self-loops weigh 1, and the weight of self-loops can be altered. Thus graphs with self-loops can be characterized by a *weighted adjacency matrix* W where $W_{xy} = A_{xy}$ for $x \neq y$ and W_{xx} being equal to the weight of self-loop on vertex x.

1.3.2 Transitivity

An *automorphism* of a graph $G = (V, E)$ is a permutation σ of the set V, such that the pair of vertices $\{x, y\} \in E$ if and only if the pair $\{\sigma(x), \sigma(y)\} \in E$.

A graph G is *vertex-transitive* if for any two distinct vertices $x, y \in V$ there is an automorphism σ such that $\sigma(x) = y$. A graph G is *edge-transitive* if for any two distinct edges $e_1, e_2 \in E$ there is an automorphism σ that maps e_1 to e_2.

A graph G is *arc-transitive* if for any two distinct arcs $a_1 = (x_1, y_1)$ and $a_2 = (x_2, y_2)$ in G, there is an automorphism σ that maps a_1 to a_2, i.e. $\sigma(x_1) = x_2$ and $\sigma(y_1) = y_2$. A graph G is *locally arc-transitive* if for any vertex x with two distinct neighbors y_1 and y_2, there exists an automorphism σ that maps the arc (x, y_1) to the arc (x, y_2).

1.3.3 Spatial search on graphs

Searching structured databases can be modelled as spatial search problems on graphs. Given an undirected graph $G = (V, E)$ and a set of marked vertices $M \subset V$, we define the following search problems.

- Detecting: Decide if there is a marked vertex in G, i.e. $|M| > 0$.
- Finding: If $|M| > 0$, find a marked vertex in M, otherwise output "No marked vertex".

In particular, if $|M| = 1$, we say the Finding problem is to find a unique marked vertex. If $|M| > 1$, we call it the case of multiple marked vertices.

1.4 Random Walks

A *random walk* is a stochastic process that describes a path that consists of a succession of random steps on graphs. This process is denoted as $\{X_0, X_1, X_2, \ldots\}$ where X_t is a random variable describing the position of the walker after t steps. At each step of the random walk, the walker randomly selects a vertex adjacent to the current position and moves to that vertex, i.e. X_{t+1} is a vertex chosen randomly from the neighbours of X_t.

To represent a random walk on a graph G with N vertices, define an $N \times N$ *transition matrix* $\mathsf{P} = \mathsf{P}(G)$, where P_{yx} is the transition probability from vertex x to vertex y. The transition matrix P can be derived from the weighted adjacency matrix W of the graph G

by computing the transition probability

$$\mathsf{P}_{yx} = \frac{W_{yx}}{\sum_k W_{kx}}.$$

We use a probability vector $\vec{v} \in \mathbb{R}^n$ to represent the probability of the walker being at each vertex of the graph. Note that in this thesis the transition matrix is column-stochastic and the probability vector is a column vector, which matches the convention for quantum computing where quantum operators are applied to quantum state vectors from the left.

Using the transition matrix, we can easily compute the future probability distribution of the random walk over all vertices in the graph. Namely, given a probability vector $\vec{v}$, the probability distribution after taking one step of random walk is $\mathsf{P}\vec{v}$. A probability distribution $\vec{\pi}$ that satisfies $\mathsf{P}\vec{\pi} = \vec{\pi}$ is called a *stationary distribution* of P, i.e. $\vec{\pi}$ is a (+1)-eigenvector of P.

1.4.1 Properties of random walks

In this thesis, we consider random walks with the following properties:

- *irreducible*: A random walk is irreducible if any vertex in the graph is reachable from any other vertex by a finite number of random walk steps. According to the Perron-Frobenius theorem [Per07, Fro12], the (+1)-eigenvector of an irreducible random walk is unique and strictly positive.

- *aperiodic*: A random walk is aperiodic if there is no integer $k > 1$ that divides the length of every directed cycle in the graph.

- *ergodic*: A random walks is ergodic if the random walk is irreducible and aperiodic. By the Perron-Frobenius theorem, an ergodic random walk P has a unique (+1)-eigenvector that corresponds to the eigenvalue equal to 1, and the remaining eigenvalues of P are strictly smaller than 1 in absolute value [Mey10]. It holds that every probability distribution $\vec{v}$ converges to the unique stationary distribution $\vec{\pi}$, i.e. $\lim_{t\to\infty} \mathsf{P}^t\vec{v} = \vec{\pi}$.

- *reversible*: An ergodic random walk P is reversible if it satisfies the detailed balance equation,

$$\mathsf{P}_{yx}\vec{\pi}_x = \mathsf{P}_{xy}\vec{\pi}_y,$$

  for any two vertices x and y in the graph. Intuitively, the reversibility says that in the stationary distribution, the probabilities moving from a vertex x to a vertex y and moving y to x are the same. Random walks on simple graphs are reversible.

1.4.2 Discriminant matrix

A random walk P could be any column-stochastic matrix but is not necessarily a real symmetric matrix, which means its eigenvectors might not be orthogonal, thus sometimes P might be hard to analyze. To address this problem, Szegedy [Sze04] introduced the *discriminant matrix* of P, defined as

$$\mathsf{D}(\mathsf{P}) = \sqrt{\mathsf{P} \circ \mathsf{P}^{\mathsf{T}}},$$

where the Hadamard product "$\circ$" and the square root are taken entry-wise, and "T" denotes the matrix transpose. If P is reversible, we can write the entries of $\mathsf{D}(\mathsf{P})$ as

$$\mathsf{D}(\mathsf{P})_{xy} = \sqrt{\mathsf{P}_{xy}\mathsf{P}_{yx}} = \sqrt{\mathsf{P}_{xy}\frac{\mathsf{P}_{xy}\vec{\pi}_y}{\vec{\pi}_x}} = \sqrt{\vec{\pi}_y}\mathsf{P}_{xy}\frac{1}{\sqrt{\vec{\pi}_x}}.$$

Then the discriminant can be expressed as a similarity transformation,

$$\mathsf{D}(\mathsf{P}) = \mathrm{diag}\left(\sqrt{\vec{\pi}}\right) \mathsf{P}\, \mathrm{diag}\left(\sqrt{\vec{\pi}}\right)^{-1},$$

which implies that P and $\mathsf{D}(\mathsf{P})$ have the same eigenvalues. The reversibility of P also implies that $\mathsf{D}(\mathsf{P})$ is a real symmetric matrix, and hence it has orthogonal eigenvectors. By the definition of $\mathsf{D}(\mathsf{P})$, we have the following correspondence between the spectra of P and $\mathsf{D}(\mathsf{P})$.

Lemma 1. *Let* $\mathsf{D}(\mathsf{P})$ *be the discriminant matrix of a reversible random walk* P*. If* $\vec{k}$ *is an eigenvector of* P *with eigenvalue* k*, then* $\mathrm{diag}(\sqrt{\vec{\pi}})^{-1}\vec{k}$ *is an eigenvector of* $\mathsf{D}(\mathsf{P})$ *with the same eigenvalue* k*. In particular, the unique* $(+1)$*-eigenvector of* $\mathsf{D}(\mathsf{P})$ *is*

$$\sqrt{\vec{\pi}} = \mathrm{diag}(\sqrt{\vec{\pi}})^{-1}\vec{\pi} = \sum_{x \in V} \sqrt{\vec{\pi}_x}|x\rangle,$$

where $\vec{\pi}$ *is the unique* $(+1)$*-eigenvector of* P*.*

We denote the eigenvalues of the discriminant $\mathsf{D}(\mathsf{P})$ by λ_k and the corresponding eigenvectors by $|\lambda_k\rangle$, where $k = 0, \ldots, N-1$. By the Perron-Frobenius theorem, if P is ergodic and reversible, all eigenvalues of $\mathsf{D}(\mathsf{P})$ are real numbers at most 1 in absolute value and 1 is a unique eigenvalue of $\mathsf{D}(\mathsf{P})$. Thus we can write eigenvalues as $\lambda_k = \cos\theta_k$, where $\theta_k \in [0, \pi)$ is the k-th *eigenphase* of $\mathsf{D}(\mathsf{P})$. Let $\lambda_0 = 1$, so $|\lambda_0\rangle = \sqrt{\vec{\pi}}$ is the unique $(+1)$-eigenvector of $\mathsf{D}(\mathsf{P})$.

1.4.3 Search via random walk

A natural approach to solve the spatial search problem on graphs is to use random walks. The following algorithm that searches via random walks finds the marked item with constant success probability.

Algorithm 1 Random Walk Search Algorithm

- Input: P, M, T.
- Output: A marked vertex or "No marked vertex".

1. Sample a vertex x from the stationary distribution $\vec{\pi}$ of the random walk P.
2. Repeat T times:
   (a) If $x \in M$, return x.
   (b) Otherwise, take one step of the random walk P.
3. Return "No marked vertex".

The random walk search algorithm is a probabalistic algorithm with one-sided error, which means it may output "No marked vertex" if there exists a marked vertex. The probability of finding a marked vertex if there exists one is the *success probability*. In Algorithm 1, the walker keeps walking until it reaches a marked vertex, and it will not move to other vertices after it reaches a marked vertex. In other words, the walk will stop at marked vertices. Hence the algorithm could be expressed as repeated applications of the *absorbing walk*. The absorbing walk P' is obtained from the random walk P by replacing all outgoing transitions from every marked vertex with self-loops, that is, $\mathsf{P}'_{xu} = \mathsf{P}_{xu}$ for all unmarked vertices u and all x, and, for any marked vertex m, $\mathsf{P}'_{mm} = 1$ and $\mathsf{P}'_{ym} = 0$ for all $y \neq m$. The success probability after taking t steps of random walk P is the sum of probabilities on marked vertices in the distribution $\mathsf{P}'^t\vec{\pi}$. Note that the self-loop on marked vertices ensures that the success probability is increasing when applying the absorbing walk P'.

To measure the complexity of the random walk algorithm, we denote the cost to *setup* by $\mathtt{S}$, the cost to *check* by $\mathtt{C}$ and the cost to *update* by $\mathtt{U}$ corresponding to step 1, 2(a) and 2(b) in Algorithm 1, respectively. The total cost of the algorithm is then $\mathtt{S} + T(\mathtt{C} + \mathtt{U})$. The intuition of the algorithm is that for an ergodic random walk P, after taking enough steps of P, the walker will eventually reach one of the marked vertices. We next need to determine a proper value of T such that the algorithm finds a marked vertex, or conclude that there is no marked vertex with a low probability of error.

1.4.4 Classical hitting time

We define the *hitting time* of a random walk based on the random walk algorithm for finding a marked vertex. Here we assume that there exists a marked vertex, i.e. $|M| > 0$.

Definition 2. The hitting time of a random walk P with respect to the set of marked vertices M, denoted by $\mathsf{HT}(\mathsf{P}, M)$, is the expected number of steps T that we need to run a random walk until it finds a marked vertex if the initially sampled vertex is unmarked.

The hitting time $\mathsf{HT}(\mathsf{P}, M)$ can be obtained using the eigenvalues and the eigenvectors of the discriminant matrix $\mathsf{D}(\mathsf{P}')$. The discriminant matrix of P' can be written in the following block form

$$\mathsf{D}(\mathsf{P}') = \sqrt{\mathsf{P}' \circ \mathsf{P}'^{\mathrm{T}}} = \begin{bmatrix} \mathsf{D}(\mathsf{P})_U & 0 \\ 0 & \mathsf{I}_M \end{bmatrix},$$

where $\mathsf{D}(\mathsf{P})_U$ is the discriminant of the transition matrix between unmarked vertices and I_M is the identity matrix on marked vertices. The largest eigenvalue of $\mathsf{D}(\mathsf{P}')$ is 1 with multiplicity $|M|$ with the corresponding eigenvectors only on marked states. Its remaining eigenvalues are real and strictly less than 1 in absolute value.

Theorem 3 (Hitting time [Sze04, KMOR16]). *The hitting time of a random walk P with respect to the set of marked vertices M is given by*

$$\mathsf{HT}(\mathsf{P}, M) = \sum_k \frac{|\langle \lambda'_k | U \rangle|^2}{1 - \lambda'_k}, \tag{1.2}$$

where $\lambda'_k \neq 1$ are the eigenvalues of $\mathsf{D}(\mathsf{P}')$ in nondecreasing order, $|\lambda'_k\rangle$ are the corresponding *eigenvectors, and*

$$|U\rangle = \frac{1}{\sqrt{1-p_M}} \sum_{x \notin M} \sqrt{\vec{\pi}_x} |x\rangle$$

with p_M being the probability of selecting a marked vertex from the stationary distribution π.

Chapter 2

Quantum Walks

Quantum walks are quantum counterparts of random walks, and they can solve searching problems asymptotically faster than random walks. There are several definitions of quantum walks, depending on the strategy for constructing the quantum walk based on the random walk. The most popular discrete quantum walk models are the *coined quantum walk* and *Szegedy's quantum walk*. In this chapter, we present and analyze these two models. We also show that these two models are equivalent under an isometry.

2.1 Coined quantum walk

The model of coined quantum walks was formally introduced by Aharonov et al. [AAKV01] and Ambainis et al. [ABN$^+$01]. In this framework, in addition to the Hilbert space spanned by the vertices of the graph, an auxiliary Hilbert space is used to specify the moving direction of the quantum walk, which is called the "coin space". The coined quantum walk has been widely applied in developing efficient quantum algorithms for several problems, including element distinctness [Amb04], the triangle problem [MSS07], and spatial search [SKW03, AKR05].

Given a d-regular graph $G = (V, E)$, we denote by N the number of vertices in G and let

$\mathcal{H}_N = \mathbb{C}^N$ be the Hilbert space spanned by vertex states $|x\rangle$ where $x \in V$. For each vertex x, fix any ordering of the d neighbors $y_1, y_2, \ldots, y_d$ of x. We refer to y_k as the k^{th} neighbor of x, and the arc (x, y_k) as the k^{th} outgoing arc of x. To each vertex we associate a coin register in the coin space $\mathcal{H}_d = \mathbb{C}^d$ spanned by the basis $\{|e_1\rangle, |e_2\rangle, \ldots, |e_d\rangle\}$. The coined quantum walk takes place in the space $\mathcal{H}_N \otimes \mathcal{H}_d$, in which the state $|x, e_k\rangle$ represents the arc (x, y_k).

The coined quantum walk is defined as

$$\mathsf{W}_{coin} = \mathsf{S}_{\text{ff}} \cdot (\mathsf{I}_N \otimes \mathsf{C}),$$

where the reflection operator $\mathsf{C} = 2|c\rangle\langle c| - \mathsf{I}_d$ with

$$|c\rangle = \frac{1}{\sqrt{d}} \sum_{k=1}^{d} |e_k\rangle$$

is a "coin-flip" acting on $\mathcal{H}_d$ and S_{ff} is the flip-flop shift operator that acts as

$$\mathsf{S}_{\text{ff}} \colon |x, e_j\rangle \mapsto |y, e_k\rangle,$$

where y is the j^{th} neighbor of x, and x is the k^{th} neighbor of y, i.e. if the walker in vertex x that points towards its neighbor y will move to vertex y and point back to vertex x after an application of S_{ff}. The unique stationary state of the coined quantum walk W_{coin} is

$$|\text{init}_{coin}\rangle = \frac{1}{\sqrt{N}} \sum_{x \in V} |x\rangle \otimes |c\rangle.$$

To search for marked vertices, the coined quantum walk requires an extra query oracle to distinguish between marked and unmarked vertices. There are many common choices for the oracle, one of which is the "SKW oracle" introduced by Shenvi, Kempe, and

Whaley [SKW03]. The SKW oracle is defined as

$$\mathsf{Q}_{SKW} = \mathsf{I}_{dN} - 2 \sum_{m \in M} |m, c\rangle\langle m, c|, \tag{2.1}$$

which reflects the marked states and acts as an identity on unmarked states. Then a quantum searching algorithm that repeatedly applies a quantum operator

$$\mathsf{A}_{coin} = \mathsf{W}_{coin} \cdot \mathsf{Q}_{SKW}.$$

is shown in Algorithm 2. Figure 2 shows the circuit of the quantum operator A_{coin}.

Algorithm 2 Quantum Walk Search Algorithm

- Input: G, M, T.
- Output: A marked vertex or "No marked vertex".

1. Prepare the initial state $|\text{init}_{coin}\rangle$.
2. Repeat T times: Apply the quantum operator A_{coin}.
3. Measure the first register of the resulting state.
4. If the measurement outcome is in M, return the outcome.
5. Otherwise return "No marked vertex".

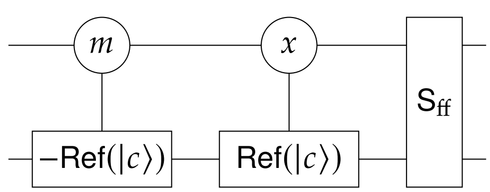

Figure 2.1: Circuit of coined quantum walk with an oracle A_{coin}.

Ambainis et al. [AKR05] proved that Algorithm 2 can find a unique marked vertex on the two-dimensional $\sqrt{N} \times \sqrt{N}$ torus in $O(\sqrt{N \log N})$ steps (i.e. $T \in O(\sqrt{N \log N})$)

with success probability in $\Omega(\frac{1}{\log N})$ and on the higher-dimensional torus in $O(\sqrt{N})$ steps with constant success probability. The two-dimensional torus is a toroidal grid graph that connects corresponding left/right and top/bottom vertex pairs with edges. More generally, the n-dimensional torus is the Cartesian product between n cycles, $\bigtimes_{i=1}^{n} C_{\sqrt[n]{N}}$. Ambainis et al. [AKR05] also simplified the result in [SKW03] that coined quantum walks can find a unique marked vertex on hypercubes in $O(\sqrt{N})$ steps with constant success probability. Their results showed that coined quantum walks find a unique marked vertex quadratically faster than random walks on tori and hypercubes.

2.2 Szegedy's quantum walk

The applications and analyses of coined quantum walks are restricted to some particular regular graphs such as hypercubes and n-dimensional tori. Szegedy generalized the coined quantum walk model by introducing a general method of constructing a quantum walk from any reversible random walk [Sze04]. Szegedy's quantum walk is a walk on the edges of the graph instead of its vertices as in random walks. Given a graph $G = (V, E)$ with N vertices, we use the state $|x\rangle$ to represent the vertex x and the state $|x, y\rangle$ to represent the arc (x, y) for any two vertices $x, y \in V$. The quantum states of Szegedy's quantum walk, which are the quantum analogue of the probability vectors of random walks, are in the Hilbert space $\mathcal{H}_N \otimes \mathcal{H}_N = \mathbb{C}^N \otimes \mathbb{C}^N$. A quantum state is marked or unmarked if the first register of the state is a marked or unmarked vertex, respectively.

For any vertex x in a random walk P, define the superposition of all neighbours of vertex x as

$$|\mathsf{P}_x\rangle = \sum_{y \in V} \sqrt{\mathsf{P}_{yx}}|y\rangle. \tag{2.2}$$

Szegedy introduced a reflection operator $\mathsf{Ref}(\mathcal{A})$ that reflects about the subspace $\mathcal{A}$

spanned by $\{|x, \mathsf{P}_x\rangle : x \in V\}$. Szegedy's quantum walk operator is defined as

$$\mathsf{W}(\mathsf{P}) = \mathsf{SWAP} \cdot \mathsf{Ref}(\mathcal{A}), \tag{2.3}$$

where the operator SWAP swaps the two registers, i.e. $\mathsf{SWAP}|x, y\rangle = |y, x\rangle$. The quantum circuit of $\mathsf{W}(\mathsf{P})$ is shown in Figure 2.2.

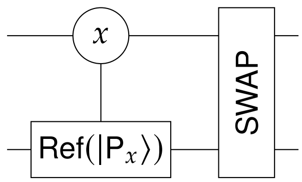

Figure 2.2: Circuit of Szegedy's quantum walk $\mathsf{W}(\mathsf{P})$.

To show the correspondence between the random walk and Szegedy's quantum walk, we define an isometry T which maps from the vertex space of the random walk P to the edge space of the quantum walk $\mathsf{W}(\mathsf{P})$,

$$\mathsf{T} = \sum_{x \in V} |x, \mathsf{P}_x\rangle\langle x|. \tag{2.4}$$

Using the isometry T, we can write the quantum walk operator $\mathsf{W}(\mathsf{P})$ as

$$\mathsf{W}(\mathsf{P}) = \mathsf{SWAP}\Big(2 \sum_{x \in V} |x, \mathsf{P}_x\rangle\langle x, \mathsf{P}_x| - \mathsf{I}\Big) = \mathsf{SWAP}\big(2\mathsf{T}\mathsf{T}^\dagger - \mathsf{I}\big),$$

and write the discriminant $\mathsf{D}(\mathsf{P})$ as

$$\begin{aligned}\mathsf{D}(\mathsf{P}) &= \sum_{x,y\in V} |y\rangle \mathsf{D}(\mathsf{P})_{yx} \langle x| = \sum_{x,y\in V} |y\rangle \sqrt{\mathsf{P}_{yx}\mathsf{P}_{xy}} \langle x| \\ &= \sum_{x,y\in V} |y\rangle\langle y|\mathsf{P}_x\rangle\langle x|\mathsf{P}_y\rangle\langle x| \\ &= \sum_{x,y\in V} |y\rangle\langle y, \mathsf{P}_y|\mathsf{SWAP}|x, \mathsf{P}_x\rangle\langle x| \\ &= \mathsf{T}^\dagger \cdot \mathsf{SWAP} \cdot \mathsf{T}.\end{aligned}$$

The stationary state of Szegedy's quantum walk $\mathsf{W}(\mathsf{P})$ is the quantum analogue of the stationary distribution $\vec{\pi}$ of P, which we denote by

$$|\text{init}\rangle = \mathsf{T}\sqrt{\vec{\pi}} = \sum_{x\in V} \sqrt{\vec{\pi}_x}|x, \mathsf{P}_x\rangle = \sum_{x,y\in V} \sqrt{\mathsf{P}_{yx}\vec{\pi}_x}|x, y\rangle. \quad (2.5)$$

The reversibility of P implies that $\mathsf{SWAP}|\text{init}\rangle = |\text{init}\rangle$ hence $\mathsf{W}(\mathsf{P})|\text{init}\rangle = |\text{init}\rangle$.

2.2.1 Spectral analysis of quantum walk

Szegedy's correspondence gives a general method to construct a quantum walk from a random walk and also relates the spectral decomposition of the quantum walk operator $\mathsf{W}(\mathsf{P})$ to that of the random walk P.

Recall that we denote the eigenvalues of the discriminant $\mathsf{D}(\mathsf{P})$ by $\lambda_k = \cos\theta_k$ and the corresponding eigenvectors by $|\lambda_k\rangle$, where $k = 0, \ldots, N-1$. To describe the spectrum and eigenspaces of the quantum walk operator, we use the isometry T to map eigenvectors of $\mathsf{D}(\mathsf{P})$ from the vertex space to the edge space. Let S_k be the subspace spanned by $\{\mathsf{T}|\lambda_k\rangle, \mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle\}$. The subspace S_k is one-dimensional if $\mathsf{T}|\lambda_k\rangle = \mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle$, and two-dimensional otherwise.

Lemma 4. *The subspace S_0 is one-dimensional and is the only* (+1)*-eigenspace of* $\mathsf{W}(\mathsf{P})$*.*

Proof. Since $|\lambda_0\rangle = \sqrt{\vec{\pi}}$ is the unique (+1)-eigenvector of $\mathsf{D}(\mathsf{P})$, we have $\mathsf{T}|\lambda_0\rangle = |\text{init}\rangle$ as the unique (+1)-eigenvector of $\mathsf{W}(\mathsf{P})$ and $\mathsf{SWAP} \cdot \mathsf{T}|\lambda_0\rangle = \mathsf{SWAP}|\text{init}\rangle = |\text{init}\rangle = \mathsf{T}|\lambda_0\rangle$. □

Lemma 5. *Subspaces S_j and S_k are orthogonal for any $j \neq k$.*

Proof. To show the orthogonality, we prove that any basis of S_j is orthogonal to that of S_k by showing their inner product is zero. First, we have the inner product

$$\langle\lambda_j|\mathsf{T}^\dagger\mathsf{T}|\lambda_k\rangle = \langle\lambda_j|\lambda_k\rangle = 0$$

since $\mathsf{D}(\mathsf{P})$ is a real symmetric matrix. Then we have the inner product

$$\langle\lambda_j|\mathsf{T}^\dagger \cdot \mathsf{SWAP} \cdot \mathsf{T}|\lambda_k\rangle = \langle\lambda_j|\mathsf{D}(\mathsf{P})|\lambda_k\rangle = \lambda_k \langle\lambda_j|\lambda_k\rangle = 0.$$

Similarly, we can also show that $\langle\lambda_j|\mathsf{T}^\dagger \cdot \mathsf{SWAP}^\dagger \cdot \mathsf{T}|\lambda_k\rangle = 0$ and $\langle\lambda_j|\mathsf{T}^\dagger \cdot \mathsf{SWAP}^\dagger \cdot \mathsf{SWAP} \cdot \mathsf{T}|\lambda_k\rangle = \langle\lambda_j|\mathsf{T}^\dagger\mathsf{T}|\lambda_k\rangle = 0$. By linearity, we prove the orthogonality between subspaces S_j and S_k for any $j \neq k$. □

Lemma 6. *The quantum walk* $\mathsf{W}(\mathsf{P})$ *preserves each subspace S_k for $k = 0, \ldots, N-1$.*

Proof. The quantum walk operator $\mathsf{W}(\mathsf{P})$ preserves the subspace S_0 since $S_0 = \text{span}\,\{\mathsf{T}|\lambda_1\rangle\}$ is the (+1)-eigenspace of $\mathsf{W}(\mathsf{P})$. For $k = 1, \ldots, N-1$, any vector in subspace S_k is a linear combination of $\mathsf{T}|\lambda_k\rangle$ and $\mathsf{SWAP} \cdot \mathsf{T}|\lambda_k\rangle$. If we show that the vectors obtained by applying $\mathsf{W}(\mathsf{P})$ to $\mathsf{T}|\lambda_k\rangle$ and $\mathsf{SWAP} \cdot \mathsf{T}|\lambda_k\rangle$ are still in the subspace S_k, which can be written as a linear combination of $\mathsf{T}|\lambda_k\rangle$ and $\mathsf{SWAP} \cdot \mathsf{T}|\lambda_k\rangle$, then by linearity, $\mathsf{W}(\mathsf{P})$ preserves the subspace S_k.

Applying $\mathsf{W(P)}$ to the vector $\mathsf{T}|\lambda_k\rangle$, we obtain

$$
\begin{aligned}
\mathsf{W(P)T}|\lambda_k\rangle &= \mathsf{SWAP}\big(2\mathsf{TT}^\dagger - \mathsf{I}\big)\mathsf{T}|\lambda_k\rangle \\
&= 2\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle - \mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle \\
&= \mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle \in S_k.
\end{aligned}
$$

Applying $\mathsf{W(P)}$ to the vector $\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle$, we obtain

$$
\begin{aligned}
\mathsf{W(P)}\cdot\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle &= \mathsf{SWAP}\big(2\mathsf{TT}^\dagger - \mathsf{I}\big)\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle \\
&= 2\mathsf{SWAP}\cdot\mathsf{TT}^\dagger\cdot\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle - \mathsf{SWAP}\cdot\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle \\
&= 2\mathsf{SWAP}\cdot\mathsf{T}\cdot\mathsf{D(P)}|\lambda_k\rangle - \mathsf{T}|\lambda_k\rangle \\
&= 2\lambda_k\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle - \mathsf{T}|\lambda_k\rangle \in S_k.
\end{aligned}
$$

Thus the subspace S_k is invariant under the action of $\mathsf{W(P)}$, for $k = 0, \dots, N-1$. □

Szegedy [Sze04] introduced a general method that gives the correspondence between spectra of $\mathsf{W(P)}$ and of $\mathsf{D(P)}$.

Theorem 7 (Spectral decomposition of $\mathsf{W(P)}$ [Sze04])**.** *The quantum walk operator* $\mathsf{W(P)}$ *has the following eigenvalues and eigenvectors:*

- *In the subspace S_0, the operator* $\mathsf{W(P)}$ *has the $(+1)$-eigenvector $|\phi_0\rangle = \mathsf{T}\sqrt{\vec{\pi}}$.*
- *In each subspace S_k with $k = 1, \dots, N-1$, the operator* $\mathsf{W(P)}$ *has eigenvalue $e^{i\theta_k}$ with eigenvector*

  $$|\phi_k^+\rangle = \mathsf{T}|\lambda_k\rangle - e^{i\theta_k}\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle = \mathsf{T}|\lambda_k\rangle + i(\mathsf{T}|\lambda_k\rangle)^\perp,$$

  and eigenvalue $e^{-i\theta_k}$ with eigenvector

  $$|\phi_k^-\rangle = \mathsf{T}|\lambda_k\rangle + e^{i\theta_k}\mathsf{SWAP}\cdot\mathsf{T}|\lambda_k\rangle = \mathsf{T}|\lambda_k\rangle - i(\mathsf{T}|\lambda_k\rangle)^\perp,$$

where $(\mathsf{T}|\lambda_k\rangle)^\perp$ *is a unit vector orthogonal to* $\mathsf{T}|\lambda_k\rangle$ *lying in the subspace* S_k.

2.2.2 Detecting via quantum absorbing walk

In order to find or detect marked vertices, the walk operator must be able to distinguish between marked and unmarked vertices. In the classical scenario, this is achieved by changing the random walk P to the absorbing walk P'. Similarly as in the quantum case, we use a quantum absorbing walk $\mathsf{W}(\mathsf{P}')$ obtained by applying Szegedy's correspondence on the absorbing walk P'.

We divide the subspace $\mathcal{A}$ into a marked subspace and an unmarked subspace:

$$\mathcal{A}_M = \operatorname{span}\{|x, \mathsf{P}_x\rangle : x \in M\},$$
$$\mathcal{A}_U = \operatorname{span}\{|x, \mathsf{P}_x\rangle : x \notin M\}.$$

Let Π_M and Π_U be projectors onto subspaces $\mathcal{A}_M$ and $\mathcal{A}_U$, respectively. A detecting algorithm using the quantum absorbing walk $\mathsf{W}(\mathsf{P}')$ is specified in Algorithm 3. The core idea of the algorithm is that the state $|\text{init}\rangle = |\overline{\text{init}}\rangle$ is a (+1)-eigenvector of the quantum operator $\mathsf{W}(\mathsf{P}) = \mathsf{W}(\mathsf{P}')$ if and only if there is no marked vertex. If there is a marked vertex, then applying $\mathsf{W}(\mathsf{P}')$ on $|\overline{\text{init}}\rangle$ changes the state so that we can distinguish between the initial state $|\text{init}\rangle$ and the resulting state $|\psi\rangle = \mathsf{W}(\mathsf{P}')^t|\overline{\text{init}}\rangle$ using the swap test. The swap test is a quantum algorithm that determines if two states are the same [BCWdW01]. It takes two quantum states $|\psi\rangle$ and $|\phi\rangle$ as input and returns 1 or 0 indicating these two states differ or not. If $|\psi\rangle = |\phi\rangle$, swap test returns 0 with certainty. Otherwise, it returns 0 with probability $\frac{1}{2} + \frac{1}{2}|\langle\phi|\psi\rangle|^2$. Thus Algorithm 3 is a probabilistic algorithm with one-sided error.

Szegedy [Sze04] proved that Algorithm 3 runs in $O(\sqrt{\mathsf{HT}})$ steps and solves the detecting problem with constant success probability. He also showed that a quantum walk algorithm

Algorithm 3 Quantum Walk Detecting Algorithm

- Input: P, M, T.
- Output: "Yes" if there exists a marked vertex, otherwise "No".

1. Prepare the initial state $|\text{init}\rangle$.
2. Measure the state $|\text{init}\rangle$ according to the projective measurement $\{\Pi_M, \Pi_U\}$.
3. If the measurement result is in Π_M, return "Yes".
4. Otherwise:
   (a) Let $|\overline{\text{init}}\rangle$ be the post-measurement state.
   (b) Randomly pick t from $\{1, \ldots, T\}$.
   (c) Apply quantum walk operator $\mathsf{W}(\mathsf{P}')$ for t steps on $|\overline{\text{init}}\rangle$ and get the resulting state $|\psi\rangle = \mathsf{W}(\mathsf{P}')^t|\overline{\text{init}}\rangle$.
   (d) If $|\psi\rangle \neq |\text{init}\rangle$, return "Yes".
   (e) Otherwise, return "No".

can find a marked vertex if the graph is vertex-transitive and there is a unique marked vertex.

Theorem 8 ([Sze04])**.** *For an ergodic and symmetric random walk* P *with a set of marked vertices* M*, Algorithm 3 detects the presence of marked vertices with constant success probability and complexity of order* $\mathsf{S} + \sqrt{\mathsf{HT}(\mathsf{P}, M)}(\mathsf{C} + \mathsf{U})$.

It is stated without proof in [MNRS12] that the quantum absorbing walk $\mathsf{W}(\mathsf{P}')$ is equivalent to the quantum operator $\mathsf{A}_{Sze} = \mathsf{W}(\mathsf{P}) \cdot \mathsf{G}$, which is Szegedy's quantum walk with an oracle. The oracle G is a reflection operator defined as

$$\mathsf{G} = \mathsf{I} - 2\Pi_M = \mathsf{I} - 2\sum_{m \in M} |m, \mathsf{P}_m\rangle\langle m, \mathsf{P}_m|. \tag{2.6}$$

Similar to the SKW oracle in coined quantum walks, the operator G reflects marked states and acts as an identity on unmarked states, which can be used to distinguish between marked and unmarked states. We can represent A_{Sze} as a quantum circuit in Figure 2.3.

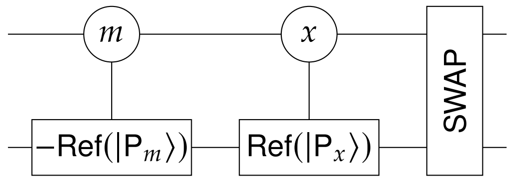

Figure 2.3: Circuit of Szegedy's quantum walk with a query $\mathsf{A}_{Sze} = \mathsf{W(P)} \cdot \mathsf{G}$.

Lemma 9. *The quantum operator* $\mathsf{A}_{Sze} = \mathsf{W(P)} \cdot \mathsf{G}$ *is equivalent to the quantum absorbing walk* $\mathsf{W(P')}$.

Proof. We first consider the operator $\mathsf{A}_{Sze} = \mathsf{W(P)} \cdot \mathsf{G}$. For an unmarked state, the operator A_{Sze} acts the same as $\mathsf{W(P)}$. For a marked state, the operator G and the reflection $\mathsf{Ref}(|m, \mathsf{P}_m\rangle)$ cancel out, which is equivalent to a phase flip, hence the operator A_{Sze} acts like $-\mathsf{SWAP}$.

By the construction of the quantum absorbing walk $\mathsf{W(P')}$, we can write it as

$$\mathsf{W(P')} = \mathsf{SWAP}\left(2\Big(\sum_{u \notin M} |u, \mathsf{P}_u\rangle\langle u, \mathsf{P}_u| + \sum_{m \in M} |m, m\rangle\langle m, m|\Big) - \mathsf{I}\right).$$

We can observe that $\mathsf{W(P')}$ acts the same as $\mathsf{W(P)}$ on unmarked states. For all marked vertice $m \in M$, the reflection acts as an identity on the state $|m, m\rangle$ and negates other marked states. Thus $\mathsf{W(P')}$ acts the same as A_{Sze} except that it does not negate the state $|m, m\rangle$. Since the sign of the amplitude on $|m, m\rangle$ does not affect the measurement, we can conclude that the operator A_{Sze} is equivalent to $\mathsf{W(P')}$. In particular, the amplitude of $|m, m\rangle$ is 0 in the initial state $|\overline{\text{init}}\rangle$, hence $\mathsf{W(P')}$ acts identically as the operator A_{Sze} when applied to the state $|\overline{\text{init}}\rangle$. □

2.3 Equivalence between Szegedy's and coined quantum walks

Consider the two quantum walks W_{coin} and $\mathsf{W}(\mathsf{P})$ on the same d-regular graph $G = (V, E)$. The search space of W_{coin} is the Hilbert space $\mathcal{H}_N \otimes \mathcal{H}_d$. The search space of $\mathsf{W}(\mathsf{P})$ is the Hilbert space $\mathcal{H}_N \otimes \mathcal{H}_N$. By Szegedy's correspondence, the quantum walk $\mathsf{W}(\mathsf{P})$ takes place within a smaller subspace $\mathbb{C}^{dN}$ of the full Hilbert space $\mathcal{H}_N \otimes \mathcal{H}_N$. We identify the subspace $\mathbb{C}^{dN}$ with $\mathcal{H}_N \otimes \mathcal{H}_d$ by defining an isometry $\mathsf{E}\colon \mathbb{C}^{dN} \to \mathcal{H}_N \otimes \mathcal{H}_d$ as follows.

For all vertices x in the graph G, and all neighbours y_k of x, let

$$\mathsf{E}|x, y_k\rangle = |x, e_k\rangle,$$

where (x, y_k) is the k^{th} arc from x.

Lemma 10. $\mathsf{W}_{coin} = \mathsf{E} \cdot \mathsf{W}(\mathsf{P}) \cdot \mathsf{E}^\dagger$.

Proof. For all vertices $x \in V$, applying the isometry E yields

$$\mathsf{E}|x, \mathsf{P}_x\rangle = |x, c\rangle,$$

which implies that

$$\mathsf{E} \cdot \mathrm{Ref}(\mathcal{A}) \cdot \mathsf{E}^\dagger = \mathsf{E} \cdot \left(2 \sum_{x \in V} |x, \mathsf{P}_x\rangle\langle x, \mathsf{P}_x| - \mathsf{I}\right) \cdot \mathsf{E}^\dagger = 2 \sum_{x \in V} |x, c\rangle\langle x, c| - \mathsf{I} = \mathsf{I}_N \otimes \mathsf{C}.$$

By definition, the S_{ff} operator is equivalent to the SWAP operator under the isometry. Thus we have

$$\mathsf{W}_{coin} = \mathsf{S}_{\mathrm{ff}} \cdot (\mathsf{I}_N \otimes \mathsf{C}) = \mathsf{E} \cdot \mathsf{SWAP} \cdot \mathrm{Ref}(\mathcal{A}) \cdot \mathsf{E}^\dagger = \mathsf{E} \cdot \mathsf{W}(\mathsf{P}) \cdot \mathsf{E}^\dagger.$$

□

Similarly, we can show that quantum operators A_{Sze} and A_{coin} are equivalent under the isometry E. We conclude that both Szegedy's quantum walk and the coined quantum walk detect the presence of marked vertices quadratically faster than random walks, and they can find a unique marked vertex on vertex-transitive graphs with symmetric transition matrices, such as hypercubes and n-dimensional tori.

Chapter 3

Finding via Quantum Walks

3.1 Quantum interpolated walk

Szegedy's quantum walk algorithm detects the presence of marked vertices quadratically faster than random walks, but it does not necessarily find marked vertices. The novel idea of *interpolated walks* proposed by Krovi et al. [KMOR16], which interpolates between a random walk and an absorbing walk, is one of the main approaches to solve the problem of finding marked vertices on general graphs.

Given a random walk P and a set of marked vertices M, we define the interpolated walk as

$$\mathsf{P}(s) = (1 - s)\mathsf{P} + s\mathsf{P}', \tag{3.1}$$

where P' is the corresponding absorbing walk and $s \in [0, 1)$ is the interpolation parameter. The interpolated walk can be interpreted as a semi-absorbing walk. Once the walker reaches a marked vertex, it will stop at the marked vertex with probability s and continue to walk with probability $1-s$. Note that $\mathsf{P}(s)$ is ergodic and reversible for any $0 \leq s < 1$ if P

is ergodic and reversible. One can also show that $\mathsf{P}(s)$ has a unique stationary distribution

$$\vec{\pi}(s) = \frac{(1-s)\vec{\pi} + s\vec{\pi}'}{(1-s) + s \cdot p_M},$$

where $\vec{\pi}$ is the stationary distribution of P, and $\vec{\pi}'$ is a (+1)-eigenvector of P' obtained by setting $\vec{\pi}'_u = 0$ for all unmarked vertices u and $\vec{\pi}'_m = \vec{\pi}_m$ for all marked vertices m.

We denote by $\mathsf{D}(\mathsf{P}(s))$ the discriminant matrix of $\mathsf{P}(s)$, and by $|\lambda_k(s)\rangle$ its eigenvector with corresponding eigenvalue $\lambda_k(s)$, where $k = 0, \ldots, N-1$. We can write eigenvalues as $\lambda_k(s) = \cos\theta_k(s)$, where $\theta_k(s) \in [0, \pi]$ is the k^{th} eigenphase of $\mathsf{D}(\mathsf{P}(s))$. By Lemma 1, the interpolated walk $\mathsf{D}(\mathsf{P}(s))$ has a unique stationary distribution

$$|\lambda_0(s)\rangle = \sqrt{\vec{\pi}(s)} = \sum_{x \in V} \sqrt{\vec{\pi}(s)_x} |x\rangle,$$

which can be written as

$$|\lambda_0(s)\rangle = \cos\varphi(s)|U\rangle + \sin\varphi(s)|M\rangle, \tag{3.2}$$

where

$$|U\rangle = \frac{1}{\sqrt{1-p_M}} \sum_{x \notin M} \sqrt{\vec{\pi}_x} |x\rangle,$$
$$|M\rangle = \frac{1}{\sqrt{p_M}} \sum_{x \in M} \sqrt{\vec{\pi}_x} |x\rangle,$$

with

$$\cos\varphi(s) = \sqrt{\frac{(1-s)(1-p_M)}{1-s(1-p_M)}}, \tag{3.3}$$

$$\sin\varphi(s) = \sqrt{\frac{p_M}{1-s(1-p_M)}}. \tag{3.4}$$

We can observe that the interpolation parameter s controls the overlap of $|\lambda_0(s)\rangle$ with $|U\rangle$ and $|M\rangle$.

Using the spectra of $\mathsf{D}(\mathsf{P}(s))$, Krovi et al. [KMOR16] defined the *interpolated hitting time* and the *extended hitting time*.

Definition 11 ([KMOR16])**.** The interpolated hitting time of $\mathsf{P}(s)$ for $s \in [0, 1)$ is defined as

$$\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)) = \sum_{k=1}^{N-1} \frac{|\langle \lambda_k(s)|U\rangle|^2}{1-\lambda_k(s)}, \tag{3.5}$$

and the extended hitting time of P with respect to M is

$$\mathsf{HT}^{+}(\mathsf{P}, M) = \lim_{s\to 1} \mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)).$$

The extended hitting time is an important quantity in analyzing the complexity of quantum walk searching algorithms. They proved that if there is a single marked vertex, i.e. $|M| = 1$, then $\mathsf{HT}^{+}(\mathsf{P}, M) = \mathsf{HT}(\mathsf{P}, M)$. However, $\mathsf{HT}^{+}(\mathsf{P}, M)$ might be greater than $\mathsf{HT}(\mathsf{P}, M)$ if $|M| > 1$ [AK15]. The relationship between interpolated hitting time and extended hitting time is exact,

$$\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)) = \frac{{p_M}^2}{(1-s(1-p_M))^2} \mathsf{HT}^{+}(\mathsf{P}, M). \tag{3.6}$$

Similar to the method of constructing Szegedy's quantum walk, we apply Szegedy's correspondence on the interpolated walk $\mathsf{P}(s)$ to construct a *quantum interpolated walk*

$$\mathsf{W}(\mathsf{P}(s)) = \mathsf{SWAP} \cdot \mathsf{Ref}(\mathcal{A}(s)).$$

The operator $\mathsf{Ref}(\mathcal{A}(s))$ is a reflection about the subspace $\mathcal{A}(s) = \mathrm{span}\{|x, \mathsf{P}(s)_x\rangle : x \in V\}$

where

$$|\mathsf{P}(s)_x\rangle = \sum_{y \in V} \sqrt{\mathsf{P}(s)_{yx}}|y\rangle$$

is a superposition over the neighbors of vertex x. The quantum circuit of $\mathsf{W}(\mathsf{P}(s))$ is depicted in Figure 3.1.

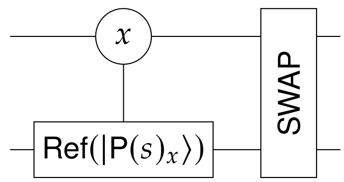

Figure 3.1: Circuit of quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$.

The isometry that maps the vertex space of interpolated walk $\mathsf{P}(s)$ to the edge space of quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$ is

$$\mathsf{T}(s) = \sum_{x \in V} |x, \mathsf{P}(s)_x\rangle\langle x|.$$

Since we construct the quantum interpolated walk using Szegedy's correspondence, the relationship between the spectra of $\mathsf{W}(\mathsf{P}(s))$ and $\mathsf{D}(\mathsf{P}(s))$ can be derived from Theorem 7.

Theorem 12 (Spectral decomposition of $\mathsf{W}(\mathsf{P}(s))$ [Sze04, KMOR16])**.** *Let $S_k(s)$ be the subspace spanned by $\{\mathsf{T}(s)|\lambda_k(s)\rangle, \mathsf{SWAP} \cdot \mathsf{T}(s)|\lambda_k(s)\rangle\}$. Then the quantum walk operator $\mathsf{W}(\mathsf{P}(s))$ has the following eigenvalues and eigenvectors:*

- *In the subspace $S_0(s)$, the operator $\mathsf{W}(\mathsf{P}(s))$ has the $(+1)$-eigenvector $|\phi_0(s)\rangle = \mathsf{T}(s)|\lambda_0(s)\rangle$.*
- *In each subspace $S_k(s)$ with $k = 1, \ldots, N-1$, the operator $\mathsf{W}(\mathsf{P})$ has eigenvalue $e^{i\theta_k(s)}$ with eigenvector*

$$|\phi_k^+(s)\rangle = \mathsf{T}(s)|\lambda_k(s)\rangle - e^{i\theta_k(s)}\mathsf{SWAP} \cdot \mathsf{T}(s)|\lambda_k(s)\rangle = \mathsf{T}(s)|\lambda_k(s)\rangle + i(\mathsf{T}(s)|\lambda_k(s)\rangle)^\perp,$$

and eigenvalue $e^{-i\theta_k(s)}$ with eigenvector

$$|\phi_k^-(s)\rangle = \mathsf{T}(s)|\lambda_k(s)\rangle + e^{i\theta_k(s)}\mathsf{SWAP}\cdot\mathsf{T}(s)|\lambda_k(s)\rangle = \mathsf{T}(s)|\lambda_k(s)\rangle - i(\mathsf{T}(s)|\lambda_k(s)\rangle)^{\perp},$$

where $(\mathsf{T}(s)|\lambda_k(s)\rangle)^{\perp}$ is a unit vector orthogonal to $\mathsf{T}(s)|\lambda_k(s)\rangle$ lying in the subspace $S_k(s)$.

3.1.1 Finding via quantum interpolated walk

Krovi et al. [KMOR16] proposed a quantum finding algorithm that applies phase estimation on the quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$, which is presented in Algorithm 4. The circuit of phase estimation is depicted in Figure 3.2.

Algorithm 4 Quantum Walk Finding Algorithm

- Input: P, M, s, t.
- Output: A marked vertex or "No marked vertex".

1. Prepare the initial state $|\text{init}\rangle$, which is the (+1)-eigenvector of $\mathsf{W}(\mathsf{P})$.
2. Measure the state $|\text{init}\rangle$ according to the projective measurement $\{\Pi_M, \Pi_U\}$.
3. If the measurement result is in Π_M, do a measurement in the vertex space and return the outcome.
4. Otherwise:
   (a) Let $|\overline{\text{init}}\rangle$ be the post-measurement state.
   (b) Attach a t-qubit register initialized as $|0^t\rangle$ to $|\overline{\text{init}}\rangle$.
   (c) Apply the phase estimation algorithm $(\mathsf{W}(\mathsf{P}(s)), t)$ on the state $|0^t\rangle|\overline{\text{init}}\rangle$.
   (d) Measure the output state on the vertex space.
   (e) If measurement outcome is in M, return the outcome.
   (f) Otherwise, return "No marked vertex".

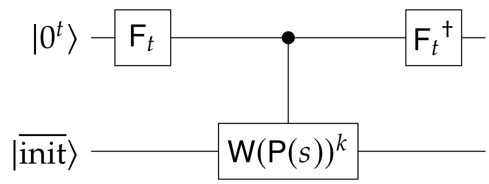

Figure 3.2: Circuit of phase estimation $(\mathsf{W}(\mathsf{P}(s)), t)$.

Here F_t is the t-dimensional Fourier transform operator that acts as

$$\mathsf{F}_t : |j\rangle \longmapsto \frac{1}{\sqrt{t}} \sum_{k=0}^{t-1} \omega_t^{jk} |k\rangle,$$

where $\omega_t = e^{\frac{2\pi i}{t}}$ is the t^{th} root of unity. The controlled-$\mathsf{W}(\mathsf{P}(s))^k$ gate applies $\mathsf{W}(\mathsf{P}(s))^k$ on the second register if the first register is $|k\rangle$, where $k = 0, 1, \ldots, 2^t - 1$. We state what the phase estimation algorithm does in Theorem 13.

Theorem 13 (Phase estimation [Kit95, CEMM98])**.** *For any unitary operator* W*, there exists a phase estimation algorithm* (W, t) *with precision* $t \in \mathbb{N}$ *that uses* 2^t *calls of* W*, and acts on eigenvectors* $|\psi\rangle$ *of* W *as*

$$|0^t\rangle|\psi\rangle \longmapsto \frac{1}{2^t} \sum_{j,k=0}^{2^t-1} e^{-\frac{2\pi i j}{2^t}(k - \frac{2^t \vartheta}{2\pi})} |k\rangle|\psi\rangle,$$

where ϑ *is the eigenphase of* W *corresponding to* $|\psi\rangle$*, i.e.* $\mathsf{W}|\psi\rangle = e^{i\vartheta}|\psi\rangle$*.*

After applying the phase estimation algorithm on the eigenvector $|\psi\rangle$ with eigenphase ϑ, the first register holds an approximation of the binary decomposition of $\frac{2^t \vartheta}{2\pi}$ and we can estimate the phase ϑ after measuring the first register. In particular, if the phase $\vartheta = 0$, which corresponds to a $(+1)$-eigenvector, then the first register is in state $|0^t\rangle$ and the estimation is exact.

In Algorithm 4, the state $|\overline{\mathrm{init}}\rangle$ is obtained by projecting to $|\mathrm{init}\rangle$ to the unmarked space, thus we can write $|\overline{\text{init}}\rangle = \mathsf{T}(s)|U\rangle$. From Equation 3.2, the unique (+1)-eigenvector of $\mathsf{W}(\mathsf{P}(s))$ can be written as

$$|\phi_0(s)\rangle = \mathsf{T}(s)|\lambda_0(s)\rangle = \cos\varphi(s)\mathsf{T}(s)|U\rangle + \sin\varphi(s)\mathsf{T}(s)|M\rangle \tag{3.7}$$

$$= \cos\varphi(s)|\overline{\text{init}}\rangle + \sin\varphi(s)\mathsf{T}(s)|M\rangle. \tag{3.8}$$

The core process of Algorithm 4 is applying the phase estimation algorithm on $|\overline{\text{init}}\rangle$ to get the (+1)-eigenvector $|\phi_0(s)\rangle$ on the second register, then measuring $|\phi_0(s)\rangle$ in the vertex space to end up with a marked vertex. To make the algorithm succeed with a high probability, we need to choose the interpolation parameter s so that $|\lambda_0(s)\rangle$ has a constant overlap with both $|U\rangle$ and $|M\rangle$. We also have to choose a proper precision t of phase estimation to distinguish between $|0^t\rangle$ and other non-zero phase states on the first register so that we can obtain $|\phi_0(s)\rangle$ in the second register with high probability.

Theorem 14 ([KMOR16]). *Let $0 \le \varepsilon_2 \le \varepsilon_1 \le \frac{1}{2}$, if*

$$\cos\varphi(s)\sin\varphi(s) \ge \varepsilon_1$$

and

$$T \ge \frac{\pi}{\sqrt{2}\varepsilon_2}\sqrt{\mathsf{HT}_{\text{ip}}(\mathsf{P}(s))}$$

where $\cos\varphi(s)$ and $\sin\varphi(s)$ are defined in Equations 3.3 and 3.4. Then Algorithm 4 with parameters s and $t = \lceil \log T \rceil$ finds a marked vertex with success probability at least

$$p_M + (1 - p_M)(\varepsilon_1 - \varepsilon_2)^2$$

and complexity of order $\mathsf{S} + T \cdot (\mathsf{U} + \mathsf{C})$.

Proof. The preparation step of Algorithm 4 in step 1 has complexity S, and the phase estimation algorithm $(\mathsf{W}(\mathsf{P}(s)), t)$ has complexity of the order $2^t \cdot (\mathtt{U} + \mathtt{C})$ according to Theorem 13. Thus the total complexity of the algorithm is of the order $\mathtt{S} + T \cdot (\mathtt{U} + \mathtt{C})$. To prove this theorem, we need to bound the success probability. The probability of measuring a marked vertex in step 3 is p_M, thus the total probability of finding a marked vertex is $p_M + (1 - p_M)q$ where q is the probability of measuring a marked vertex in step 4(d). It remains to show that $q \geq (\varepsilon_1 - \varepsilon_2)^2$.

We decompose $|U\rangle$ into the basis of $\mathsf{D}(\mathsf{P}(s))$ for scalars $\alpha_k(s)$,

$$|U\rangle = \sum_{k=0}^{N-1} \alpha_k(s)|\lambda_k(s)\rangle. \tag{3.9}$$

From Theorem 12, we observe that

$$\mathsf{T}(s)|\lambda_k(s)\rangle = \frac{1}{\sqrt{2}}(|\phi_k^+(s)\rangle + |\phi_k^-(s)\rangle),$$

for $k = 1, \ldots, N-1$. Thus we can write $|\overline{\text{init}}\rangle$ as

$$\begin{aligned} |\overline{\text{init}}\rangle = \mathsf{T}(s)|U\rangle &= \sum_{k=0}^{N-1} \alpha_k(s)\mathsf{T}(s)|\lambda_k(s)\rangle \\ &= \alpha_0(s)|\phi_0(s)\rangle + \frac{1}{\sqrt{2}}\sum_{k=1}^{N-1} \alpha_k(s)(|\phi_k^+(s)\rangle + |\phi_k^-(s)\rangle). \end{aligned} \tag{3.10}$$

From Theorem 13, we see that the phase estimation $(\mathsf{W}(\mathsf{P}(s)), t)$ acts as follows:

$$|0^t\rangle|\phi_0(s)\rangle \mapsto |0^t\rangle|\phi_0(s)\rangle,$$
$$|0^t\rangle|\phi_k^\pm(s)\rangle \mapsto |\xi_k^\pm(s)\rangle|\phi_k^\pm(s)\rangle,$$

where $|\xi_k^{\pm}(s)\rangle$ is a vector that estimates the phase of $|\phi_k^{\pm}(s)\rangle$,

$$|\xi_k^{\pm}(s)\rangle = \frac{1}{2^t}\sum_{j,k=0}^{2^t-1} e^{-\frac{2\pi i j}{2^t}(k-\frac{2^t\theta_k(s)}{2\pi})}|k\rangle.$$

Thus the state after applying phase estimation on $|0^t\rangle|\overline{\text{init}}\rangle$ is

$$|\Psi\rangle = \alpha_0(s)|0^t\rangle|\phi_0(s)\rangle + \frac{1}{\sqrt{2}}\sum_{k=1}^{N-1}\alpha_k(s)(|\xi_k^+(s)\rangle|\phi_k^+(s)\rangle + |\xi_k^-(s)\rangle|\phi_k^-(s)\rangle).$$

We denote $\delta_k^{\pm}$ the overlap between $|0^t\rangle$ and $|\xi_k^{\pm}\rangle$,

$$\delta_k^{\pm} = \langle 0^t|\xi_k^{\pm}\rangle = \frac{1}{2^t}\sum_{j=0}^{2^t-1} e^{\pm i\theta_k(s)j}. \tag{3.11}$$

Recall that q is the probability of obtaining a marked vertex by measuring the second register of $|\Psi\rangle$. To make q as large as possible, we need to choose a large enough precision t to make $\delta_k^{\pm}$ small so that $|0^t\rangle$ and $|\xi_k^{\pm}\rangle$ can be distinguished with a high probability. Then we can get state $|0^t\rangle$ in the first register and state $|\phi_0(s)\rangle$ in the second register with a high probability. To show the relationship between q and t, we start with the lower bound of q.

$$\begin{aligned}
\sqrt{q} &= \|(\mathrm{I}\otimes\Pi_M)|\Psi\rangle\|_2 \\
&\geq \|(|0^t\rangle\langle 0^t|\otimes\Pi_M)|\Psi\rangle\|_2 \\
&\geq \|\alpha_0(s)\Pi_M|\phi_0(s)\rangle\|_2 - \frac{1}{\sqrt{2}}\left\|\Pi_M\sum_{k=1}^{N-1}\alpha_k(s)(\delta_k^+|\phi_k^+(s)\rangle + \delta_k^-|\phi_k^-(s)\rangle)\right\|_2 \\
&\geq \|\alpha_0(s)\Pi_M|\phi_0(s)\rangle\|_2 - \frac{1}{\sqrt{2}}\left\|\sum_{k=1}^{N-1}\alpha_k(s)(\delta_k^+|\phi_k^+(s)\rangle + \delta_k^-|\phi_k^-(s)\rangle)\right\|_2
\end{aligned}$$

From Equation 3.8, we find that $\alpha_0(s) = \langle\phi_0(s)|\overline{\text{init}}\rangle = \cos\varphi(s)$ and $\|\Pi_M|\phi_0(s)\rangle\|_2 =$

$\sin\varphi(s)$. Note that eigenvectors $|\phi_k^+(s)\rangle$ are orthonormal, and $\delta_k^\pm$ are complex conjugates, thus we have

$$\sqrt{q} \geq \cos\varphi(s)\sin\varphi(s) - \sqrt{\sum_{k=1}^{N-1} |\alpha_k(s)|^2 \delta_k^2}, \tag{3.12}$$

where $\delta_k = |\delta_k^\pm|$. We use the closed-from formula of geometric series in Equation 3.11,

$$\delta_k^2 = \left| \frac{1}{2^t} \sum_{j=0}^{2^t-1} e^{i\theta_k(s)j} \right|^2 = \frac{1}{2^{2t}} \left| \frac{1 - e^{i\theta_k(s)2^t}}{1 - e^{i\theta_k(s)}} \right|^2 = \frac{\sin^2\left(\frac{2\theta_k(s)}{2} 2^t\right)}{2^{2t} \sin^2\left(\frac{2\theta_k(s)}{2}\right)}.$$

Since $\sin\frac{\theta_k(s)}{2} \geq \frac{\theta_k(s)}{\pi}$ for $\theta_k(s) \in [0, \pi]$, we get the upper bound of δ_k^2,

$$\delta_k^2 \leq \frac{1}{2^{2t} \frac{\theta_k^2(s)}{\pi^2}} \leq \frac{\pi^2}{T^2 \theta_k^2(s)}. \tag{3.13}$$

By the definition of interpolated hitting time in Definition 11, we have

$$\begin{aligned} \mathsf{HT}_{\text{ip}}(\mathsf{P}(s)) &= \sum_{k=1}^{N-1} \frac{|\langle \lambda_k(s)|U\rangle|^2}{1 - \lambda_k(s)} \\ &= \sum_{k=1}^{N-1} \frac{|\alpha_k(s)|^2}{1 - \cos\theta_k(s)} \\ &= \sum_{k=1}^{N-1} \frac{|\alpha_k(s)|^2}{2\sin^2\left(\frac{\theta_k(s)}{2}\right)} \\ &\geq 2 \sum_{k=1}^{N-1} \frac{|\alpha_k(s)|^2}{\theta_k^2(s)}, \end{aligned} \tag{3.14}$$

where we write $\lambda_k(s)$ as $\cos\theta_k(s)$ and substitute $\langle \lambda_k(s)|U\rangle = \alpha_k(s)$ according to Equation 3.9. Combining Equations 3.13 and 3.14, we get

$$\sum_{k=1}^{N-1} |\alpha_k(s)|^2 \delta_k^2 \leq \sum_{k=1}^{N-1} |\alpha_k(s)|^2 \frac{\pi^2}{T^2 \theta_k^2(s)} = \frac{\pi^2}{T^2} \sum_{k=1}^{N-1} \frac{|\alpha_k(s)|^2}{\theta_k^2(s)} \leq \frac{\pi^2}{2} \frac{\mathsf{HT}_{\text{ip}}(\mathsf{P}(s))}{T^2}.$$

Inserting the inequality above into Equation 3.12, we get

$$\sqrt{q} \geq \cos\varphi(s)\sin\varphi(s) - \frac{\pi}{\sqrt{2}}\frac{\sqrt{\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s))}}{T}. \tag{3.15}$$

Our assumptions in this theorem are that $\cos\varphi(s)\sin\varphi(s) \geq \varepsilon_1$ and $T \geq \frac{\pi}{\sqrt{2}\varepsilon_2}\sqrt{\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s))}$, thus $\sqrt{q} \geq \varepsilon_1 - \varepsilon_2$. □

Intuitively, we want to choose a interplation parameter s that maximizes $\cos\varphi(s)\sin\varphi(s)$, since it will increase the success probability according to Equation 3.15. The maximal value of $\cos\varphi(s)\sin\varphi(s)$ is achieved when $\cos\varphi(s) = \sin\varphi(s) = \frac{1}{\sqrt{2}}$. From Equations 3.3 and 3.4, the optimal s can be expressed as a function of p_M,

$$s(p_M) = 1 - \frac{p_M}{1 - p_M}. \tag{3.16}$$

By Equation 3.6, we have $\mathsf{HT}^+(\mathsf{P}, M) \geq \mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s))$. If there is a unique marked vertex, we know $\mathsf{HT}(\mathsf{P}, M) = \mathsf{HT}^+(\mathsf{P}, M)$, thus we can pick $T \geq \frac{\pi}{\sqrt{2}\varepsilon_2}\sqrt{\mathsf{HT}(\mathsf{P}, M)}$ so that Algorithm 4 finds the unique marked vertex with constant success probability.

Theorem 15 ([KMOR16]). *For an ergodic and reversible random walk* P *with a unique marked vertex* m*, Algorithm 4 finds the marked vertex* m *with constant success probability and complexity of order* $\mathsf{S} + \sqrt{\mathsf{HT}(\mathsf{P}, \{m\})}(\mathsf{C} + \mathsf{U})$.

3.1.2 Quantum hitting time

We define the *quantum hitting time* based on the complexity of the phase estimation algorithm. The definition of quantum hitting time is not restricted to quantum walks since we can apply phase estimation on any unitary operator.

Definition 16 ([DH17]). The quantum hitting time of a real unitary W from a state $|w\rangle$ is

$$\mathsf{QHT}(\mathsf{W}, |w\rangle) = \sqrt{\sum_k \left|\langle\psi_k^\pm|w\rangle\right|^2 \frac{1}{\vartheta_k^2}}$$

where $|\psi_k^\pm\rangle$ are eigenvectors of W with non-zero phases, i.e. $\phi_k^\pm = e^{\pm i\vartheta_k}$ and $\vartheta_k \neq 0$.

Definition 16 has an algorithmic interpretation. Namely, $\mathsf{QHT}(\mathsf{W}, |w\rangle)$ is the complexity of phase estimation to extract the (+1)-eigenvector of W starting from $|w\rangle$. We show this by analyzing the error probability of phase estimation. Recall that $\delta_k^\pm$ is the overlap between $|0^t\rangle$ and $|\xi_k^\pm\rangle$ as defined in Equation 3.11. Applying phase estimation (W, t) on state $|0^t\rangle|w\rangle$, the error probability of not getting the (+1)-eigenvector $|\psi_0\rangle$ on the second register when having $|0^t\rangle$ on the first register can be expressed as

$$\mathrm{P}_{err} = \sum_k \left|\langle\psi_k^\pm|w\rangle\right|^2 \delta_k^2 \leq \sum_k \frac{\pi^2\left|\langle\psi_k^\pm|w\rangle\right|^2}{T^2\vartheta_k^2}.$$

Letting $\mathrm{P}_{err} \leq c$ for some constant c, the number of steps of applying W in phase estimation is

$$T \geq \frac{\pi}{\sqrt{c}}\sqrt{\sum_k \left|\langle\psi_k^\pm|w\rangle\right|^2 \frac{1}{\vartheta_k^2}} \in \Theta\big(\mathsf{QHT}(\mathsf{W}, |w\rangle)\big).$$

Dohotaru and Høyer [DH17] defined another quantum hitting time which involves cotangents of the eigenphases.

Definition 17 ([DH17]). The *cotangent quantum hitting time* of a real unitary W from a state $|w\rangle$ is

$$\mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}, |w\rangle) = \sqrt{\sum_k \left|\langle\psi_k^\pm|w\rangle\right|^2 \cot^2\frac{\vartheta_k}{2}}.$$

where $|\psi_k^\pm\rangle$ are eigenvectors of W with non-zero phases, i.e. $\phi_k^\pm = e^{\pm i\vartheta_k}$ and $\vartheta_k \neq 0$.

Dohotaru and Høyer [DH17] proved that the cotangent quantum hitting time $\mathsf{QHT}_{\mathrm{cot}}$

is of the same order as QHT. In this thesis, we use the definition of cotangent hitting time since there is an exact relationship between $\mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}'), |\overline{\mathrm{init}}\rangle)$ and $\mathsf{HT}(\mathsf{P}, M)$. From now on, we use the cotangent definition when we refer to quantum hitting time.

Lemma 18. *Given a random walk* P *with a marked subset* M *and the corresponding quantum walk* $\mathsf{W}(\mathsf{P}')$,

$$\mathsf{QHT}^2_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}'), |\overline{\mathrm{init}}\rangle) = 2\mathsf{HT}(\mathsf{P}, M) - 1.$$

Proof. We decompose the vector $|U\rangle$ into the spectra of $\mathsf{D}(\mathsf{P}')$. Since $|U\rangle$ does not overlap with marked states, which means it does not overlap with (+1)-eigenvectors of $\mathsf{D}(\mathsf{P}')$, we have

$$|U\rangle = \sum_k \alpha'_k |\lambda'_k\rangle,$$

where $|\lambda'_k\rangle$ are eigenvectors of $\mathsf{D}(\mathsf{P}')$ with eigenvalues $\lambda'_k = \cos\theta'_k \neq 1$. By Szegedy's correspondence and $|\overline{\mathrm{init}}\rangle = \mathsf{T}|U\rangle$, we have

$$\begin{aligned}
\mathsf{QHT}^2_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}'), |\overline{\mathrm{init}}\rangle) &= \sum_k \left|\langle \phi'^{\pm}_k | \overline{\mathrm{init}}\rangle\right|^2 \cot^2 \frac{\theta'_k}{2} \\
&= \sum_k |\alpha'_k|^2 \frac{\cos\theta'_k + 1}{1 - \cos\theta'_k} \\
&= \sum_k \left|\langle \lambda'_k | U\rangle\right|^2 \left(\frac{2}{1-\lambda'_k} - 1\right) \\
&= 2\sum_k \frac{|\langle \lambda'_k | U\rangle|^2}{1-\lambda'_k} - \sum_k \left|\langle \lambda'_k | U\rangle\right|^2 \\
&= 2\mathsf{HT}(\mathsf{P}, M) - 1.
\end{aligned}$$

□

Similarly, we can relate the quantum hitting time $\mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\mathrm{init}}\rangle)$ to the interpolated hitting time $\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s))$.

Lemma 19. *Given an interpolated walk* $\mathsf{P}(s)$ *and the corresponding quantum interpolated walk* $\mathsf{W}(\mathsf{P}(s))$*,*

$$\mathsf{QHT}^2_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\mathrm{init}}\rangle) = 2\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)) - 1 + \cos^2\varphi(s),$$

where $\cos\varphi(s)$ *is defined in Equation 3.3.*

Proof. By the decomposition of $|U\rangle$ and $|\overline{\mathrm{init}}\rangle$ in Equations 3.9 and 3.10,

$$\begin{aligned}
\mathsf{QHT}^2_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\mathrm{init}}\rangle) &= \sum_{k=1}^{N-1} \left|\langle\phi_k^{\pm}(s)|\overline{\mathrm{init}}\rangle\right|^2 \cot^2\frac{\theta_k(s)}{2} \\
&= \sum_{k=1}^{N-1} |\alpha_k(s)|^2 \frac{\cos\theta_k(s)+1}{1-\cos\theta_k(s)} \\
&= \sum_{k=1}^{N-1} \left|\langle\lambda_k(s)|U\rangle\right|^2 \left(\frac{2}{1-\lambda_k(s)} - 1\right) \\
&= 2\sum_{k=1}^{N-1} \frac{|\langle\lambda_k(s)|U\rangle|^2}{1-\lambda_k(s)} - \sum_{k=1}^{N-1} \left|\langle\lambda_k(s)|U\rangle\right|^2 \\
&= 2\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)) - (1 - \left|\langle\lambda_0(s)|U\rangle\right|^2) \\
&= 2\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)) - 1 + \cos^2\varphi(s).
\end{aligned}$$

□

3.2 Controlled quantum walk

Dohotaru and Høyer [DH17] introduced a new abstract search framework called *controlled quantum amplification*, which we denote by U. Like the quantum interpolated walk, controlled quantum amplification circumvents the limitation of Szegedy's quantum walk, but it is more general since it can be applied to any abstract search algorithm. Using the framework of controlled quantum amplification, we can simulate Grover's quantum search algorithm [Gro96], amplitude amplification [BHMT02], Szegedy's quantum walks, and quantum interpolated walks.

The quantum circuit of U is shown in Figure 3.3. Here W is an arbitrary unitary operator

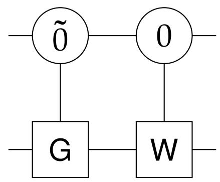

Figure 3.3: Circuit of controlled quantum amplitude amplification U.

and G is a reflection operator defined as $\mathsf{G} = \mathsf{I} - 2\Pi_g$, where Π_g is a projection on a target state $|g\rangle$. In particular, if W is the quantum walk operator $\mathsf{W}(\mathsf{P})$ and G is the query oracle defined in Equation 2.6, then the operator U is called *controlled quantum walk*.

The action of operators W and G are controlled by an extra qubit parametrized by an angle $\tilde{\theta}$. The basis $\{|\tilde{0}\rangle, |\tilde{1}\rangle\}$ is obtained from rotating the computational basis $\{|0\rangle, |1\rangle\}$ by the angle $\tilde{\theta}$, where

$$|\tilde{0}\rangle = \cos\tilde{\theta}|0\rangle + \sin\tilde{\theta}|1\rangle \quad \text{and} \quad |\tilde{1}\rangle = -\sin\tilde{\theta}|0\rangle + \cos\tilde{\theta}|1\rangle.$$

The algorithm of the controlled quantum walk starts with the state $|\text{init}\rangle$, which is the unique (+1)-eigenvector of $\mathsf{W}(\mathsf{P})$. It does a projective measurement in Π_M and Π_U. If the result is in the marked subspace, it outputs the target state $|g\rangle$. Otherwise, it attaches an extra qubit initialized to $|0\rangle$ to the measurement result $|\overline{\text{init}}\rangle$. Then it applies phase estimation on the controlled quantum walk U to the state $|0, \overline{\text{init}}\rangle$ and produces a (+1)-eigenvector of U that has constant overlap with $|\tilde{1}, g\rangle$.

Lemma 20 ([DH17])**.** *The unique* (+1)*-eigenvector of the controlled quantum walk* U *is the (unnormalized) state*

$$|u_0\rangle = \frac{1}{\sqrt{2}}|\tilde{1}, g\rangle - \frac{1}{\sqrt{2}}\sin\tilde{\theta}\frac{\cos\theta}{\sin\theta}|0, \overline{\text{init}}\rangle,$$

where $\sin^2\theta = p_M = |\langle g|\text{init}\rangle|^2$.

To increase the success probability of finding a marked vertex, we want the (+1)-eigenvector $|u_0\rangle$ has a constant overlap with both the initial state $|0, \overline{\text{init}}\rangle$ and the target state $|\tilde{1}, g\rangle$. Thus we choose an optimal $\tilde{\theta}$ such that $\sin\tilde{\theta} = \frac{\sin\theta}{\cos\theta}$.

Theorem 21 ([DH17])**.** *For an ergodic and reversible random walk* P *with a unique marked vertex, there exists a quantum algorithm that, using the controlled quantum walk* U *finds the marked vertex with constant success probability and complexity of order* $\mathsf{S} + \mathsf{QHT}_{\cot}(\mathsf{A}, |\overline{\text{init}}\rangle)(\mathsf{C} + \mathsf{U})$.

3.2.1 Simulation of quantum interpolated walks

From the construction of controlled quantum walks, the reflection operator G is activated if the first register is $|\tilde{0}\rangle$ and the quantum walk operator $\mathsf{W(P)}$ is activated if the first register is $|0\rangle$. Since we apply the controlled quantum walk U starting on the state $|0, \overline{\text{init}}\rangle$, we can consider U as a superposition of $\mathsf{W(P)}$ and $\mathsf{A}_{Sze} = \mathsf{W(P)} \cdot \mathsf{G}$. From Lemma 9, one can interpret U as an interpolation between $\mathsf{W(P)}$ and $\mathsf{W(P')}$.

Dohotaru and Høyer [DH17] showed that the controlled quantum walk simulates the quantum interpolated walk with an interpolation parameter s, by choosing the angle $\tilde{\theta}$ such that

$$\sin\tilde{\theta} = \sqrt{1-s}.$$

The optimal value of $\tilde{\theta}$, which is $\arcsin\left(\frac{\sin\theta}{\cos\theta}\right)$, corresponds to the optimal value of s that is $1 - \frac{p_M}{1-p_M}$ given by Equation 3.16.

Theorem 22 ([DH17])**.** *Given a quantum interpolated walk* $\mathsf{W(P}(s))$ *with* $0 \leq s < 1$, *there is an inner-product preserving map* E_s *from space of* $\mathsf{W(P}(s))$ *to the space of a controlled quantum walk* U, *such that* $\mathsf{E}_s \cdot \mathsf{W(P}(s)) = \mathsf{U} \cdot \mathsf{E}_s$.

Chapter 4

Lackadaisical Quantum Walks

Coined quantum walks are commonly applied on regular graphs without self-loops. The idea of adding self-loops was first applied by Ambainis et al. [AKR05], who showed that a coined quantum walk on a complete graph with a self-loop on every vertex corresponds to Grover's algorithm. Wong then generalized this model and proposed the *lackadaisical quantum walk* [Won15]. The lackadaisical quantum walk is a quantum analogue of the lazy random walk, which adds a self-loop of weight ℓ to each vertex.

Given a d-regular undirected graph $G = (V, E)$, by adding a self-loop of weight ℓ to every vertex, the coin Hilbert space $\mathcal{H}_{d+1}$ is spanned by $\{|e_1\rangle, |e_2\rangle, \ldots, |e_d\rangle, |\circlearrowleft\rangle\}$. The lackadaisical quantum walk is defined as

$$\mathsf{A}_{lazy} = \mathsf{W}_{lazy} \cdot \mathsf{Q}. \tag{4.1}$$

Here W_{lazy} is the quantum walk operator defined as $\mathsf{W}_{lazy} = \mathsf{S}_{\text{ff}} \cdot (\mathsf{I}_N \otimes \mathsf{C})$, where the operator $\mathsf{C} = 2|c\rangle\langle c| - \mathsf{I}_{d+1}$ with

$$|c\rangle = \frac{1}{\sqrt{d+\ell}}\left(|e_1\rangle + |e_2\rangle + \cdots + |e_d\rangle + \sqrt{\ell}|\circlearrowleft\rangle\right) \tag{4.2}$$

is the coin flip for a weighted graph, and S_{ff} is the flip-flop shift operator defined as

$$\mathsf{S}_{\text{ff}}\colon \begin{cases} |x, e_i\rangle & \mapsto \quad |y, e_j\rangle \\ |x, \circlearrowleft\rangle & \mapsto \quad |x, \circlearrowleft\rangle, \end{cases}$$

where y is the i^{th} neighbor of x, and x is the j^{th} neighbor of y. The operator Q is a "Grover oracle" defined as

$$\mathsf{Q} = \left(\mathsf{I}_N - 2\sum_{m\in M} |m\rangle\langle m|\right) \otimes \mathsf{I}_{d+1}, \tag{4.3}$$

which negates all marked states and acts as an identity on unmarked states. Note that the choice of oracle here is different from the coined quantum walk, as Wong showed that the Grover oracle Q performs better than the SKW oracle Q_{SKW} in lackadaisical quantum walks [Won15, Won18b].

The unique (+1)-eigenvector of W_{lazy} is

$$|\text{init}_{lazy}\rangle = \frac{1}{\sqrt{N}} \sum_{x\in V} |x\rangle \otimes |c\rangle.$$

Compared to the coined quantum walk search algorithm 2, we prefer to start with a slightly different initial state

$$|\overline{\text{init}}_{lazy}\rangle = \frac{1}{\sqrt{N - |M|}} \sum_{x\notin M} |x\rangle \otimes |c\rangle, \tag{4.4}$$

which is the projection of $|\text{init}_{lazy}\rangle$ onto the unmarked subspace. We have seen this substitution in Szegedy's Algorithm 3. The choice of the initial state is also motivated by the relationship between quantum hitting time and hitting time in Lemma 18.

The algorithm of the lackadaisical quantum walk starts with the state $|\text{init}_{lazy}\rangle$, which is the unique (+1)-eigenvector of W_{lazy}. It does a projective measurement with respect to $\{\Pi_M, \Pi_U\}$. If the result is in the marked subspace, it outputs a marked state. Otherwise, it applies the lackadaisical quantum walk A_{lazy} on the state $|\overline{\text{init}}_{lazy}\rangle$ for T times and measures the resulting state to get a marked vertex.

4.1 Known results

4.1.1 A unique marked vertex

The lackadaisical quantum walk with a unique marked vertex has been studied on several classes of graphs.

First, the complete graph was studied by Ambainis et al. [AKR05] and Wong [Won15, Won17, Won18a], who proved analytically that the lackadaisical quantum walk with $\ell = 1$ finds a unique marked vertex in $O(\sqrt{N})$ steps with probability close to 1. They also show the equivalence between the lackadaisical quantum walk on complete graphs and Grover's algorithm.

Second, the $\sqrt{N} \times \sqrt{N}$ torus was independently studied by Wong [Won18b] and Wang et al. [WZWY17]. They both showed that the lackadaisical quantum walk finds a unique marked vertex in $O(\sqrt{N \log N})$ steps with probability close to 1 in numerical results. The value of ℓ is $\frac{4}{N}$ in Wong [Won18b] and $\frac{4}{N-1}$ in Wang et al. [WZWY17]. The result is strongly supported by the experiments, but with no analytical proof of the complexity and success probability, the result is stated as a conjecture.

Third, the cycle was studied by Giri and Korepin [GK20], who numerically showed that by setting $\ell = \frac{2}{N}$, the lackadaisical quantum walk finds a unique marked vertex with probability at least a constant.

Fourth, regular complete bipartite graphs were studied by Rhodes and Wong [RW19]. They proved analytically that the lackadaisical quantum walk with $\ell = \frac{1}{2}$ finds a unique marked vertex in $O(\sqrt{N})$ steps with probability close to 1.

Fifth, in a recent paper, Rhodes and Wong [RW20] study a collection of graphs. Their collection is a rich sample of vertex-transitive graphs, comprised of the following instances and classes of graphs: arbitrary-dimensional cubic lattices, Paley graphs, the two Latin square graphs with strongly regular parameters $(9, 6, 3, 6)$ and $(1024, 93, 32, 6)$, triangular graphs, Johnson graphs, and hypercubes. They numerically show that by setting $\ell = \frac{d}{N}$, the lackadaisical quantum walk finds a unique marked vertex on d-regular vertex-transitive graphs in $O(\sqrt{\mathsf{HT}})$ steps with probability at least a constant. They propose that this holds for all vertex-transitive graphs with a unique marked vertex, and they propose that the weight of self-loop $\ell = \frac{d}{N}$ optimally boosts the success probability.

From the numerical results shown above, one can see that adding self-loops yields an improvement on the success probability over the loopless coined quantum walks. The complexity and success probability of lackadaisical quantum walks match the best known quantum search algorithms on those graphs. Although quantum walks with success probability close to 1 and those with constant success probability have the same order of complexity, having higher success probability is still beneficial. Since quantum walks have one-sided error, we may need to repeatedly run the quantum walk algorithm as a subroutine to find a marked vertex. Having a subroutine with higher success probability reduces the total cost of the search algorithm.

4.1.2 Multiple marked vertices

Lackadaisical quantum walks with multiple marked vertices are commonly studied on 2-dimensional tori.

When there are multiple marked vertices, the lackadaisical quantum walk may fail in finding a marked vertex. Nahimovs [Nah19] proved that on a $\sqrt{N} \times \sqrt{N}$ torus with *two* marked vertices placed adjacent to each other, the lackadaisical quantum walk has a stationary state that is close to the initial state, which implies that the walk finds a marked vertex with probability no bigger than $O(1/N)$. We respectfully remark that we discovered this result independently.

Consider a 2-dimensional $\sqrt{N} \times \sqrt{N}$ torus with a self-loop of weight ℓ on every vertex, and with two adjacent marked vertices m_1 and m_2 located at (x, y) and $(x+1, y)$, respectively. The coin space is spanned by $\{|\uparrow\rangle, |\downarrow\rangle, |\leftarrow\rangle, |\rightarrow\rangle, |\circlearrowleft\rangle\}$, where the basis indicates the direction of edges from a vertex.

Define an unnormalized state

$$|\psi\rangle = |\text{init}_{lazy}\rangle - \alpha(4+\ell)\big(|m_1, \rightarrow\rangle + |m_2, \leftarrow\rangle\big),$$

where

$$\alpha = \frac{1}{\sqrt{(4+\ell)N}}$$

is the amplitude of each state in $|\text{init}_{lazy}\rangle$ other than self-loops.

Lemma 23 ([Nah19])**.** *The (unnormalized) state $|\psi\rangle$ is a $(+1)$-eigenvector of the lackadaisical quantum walk operator with a Grover oracle, i.e. $\mathsf{A}_{lazy}|\psi\rangle = |\psi\rangle$.*

Proof. Consider the state $|\psi\rangle$: the amplitude of the self-loop on each vertex is $\alpha\sqrt{\ell}$, the amplitude of $|m_1, \rightarrow\rangle$ and $|m_2, \leftarrow\rangle$ is $-\alpha(3+\ell)$, and the amplitude of other states is α.

By definition, the Grover oracle Q acts as an identity on the unmarked states and negates the marked states m_1 and m_2. The coin-flip operator $\mathsf{C} = 2|c\rangle\langle c| - \mathsf{I}_{d+1}$ acts as an identity on the coin of unmarked states. By direct calculation, the operator C negates the coin of the marked states m_1 and m_2 in $|\psi\rangle$. Thus the operator $(\mathsf{I}_N \otimes \mathsf{C}) \cdot \mathsf{Q}$ acts as an identity on the state $|\psi\rangle$. By symmetry, the flip-flop shift S_{ff} does not change the state $|\psi\rangle$. Therefore, the state $|\psi\rangle$ is a $(+1)$-eigenvector of A_{lazy}. $\square$

Lemma 24 ([Nah19])**.** *On a $\sqrt{N} \times \sqrt{N}$ torus with a self-loop of weight $\ell = \frac{4}{N}$ on each vertex where there are two adjacent marked vertices m_1 and m_2, applying any number of steps of the lackadaisical quantum walk A_{lazy} on the initial state $|\text{init}_{lazy}\rangle$, the success probability of finding a* *marked vertex is $O(1/N)$.*

Proof. Write the initial state as

$$|\text{init}_{lazy}\rangle = |\psi\rangle + \alpha(4+\ell)\big(|m_1, \rightarrow\rangle + |m_2, \leftarrow\rangle\big).$$

By Lemma 23, the only part of the initial state changed by A_{lazy} is

$$|\phi\rangle = \alpha(4+\ell)\big(|m_1, \rightarrow\rangle + |m_2, \leftarrow\rangle\big).$$

Consider all marked states in the stationary state $|\psi\rangle$: the amplitude of the self-loops on marked vertices m_1 and m_2 is $\alpha\sqrt{\ell}$, the amplitude of $|m_1, \rightarrow\rangle$ and $|m_2, \leftarrow\rangle$ is $-\alpha(3+\ell)$, and the amplitude of other six marked states is α. Since the quantum walk operator A_{lazy} is unitary, the success probability of finding a marked vertex is

$$\begin{aligned}\Pr_{succ} &\leq 6\alpha^2 + 2(\alpha\sqrt{\ell})^2 + 2(-\alpha(3+\ell))^2 + \||\phi\rangle\|^2 \\ &= 6\alpha^2 + 2(\alpha\sqrt{\ell})^2 + 2(-\alpha(3+\ell))^2 + 2(\alpha(4+\ell))^2. \end{aligned} \tag{4.5}$$

Since $\ell = \frac{4}{N}$ and $\alpha = \frac{1}{\sqrt{(4+\ell)N}} = \frac{1}{\sqrt{4N+4}}$, each summand in Equation 4.5 is $O(1/N)$. Therefore the success probability of finding a marked vertex is $\Pr_{succ} \in O(1/N)$. □

The result implies that the lackadaisical quantum walk fails to find a marked vertex on a $\sqrt{N} \times \sqrt{N}$ torus if marked vertices are arranged in a $2k \times j$ or $k \times 2j$ rectangular block for $k, j \in \mathbb{N}$. Remark that this limitation of the lackadaisical quantum walk is not because of the self-loops but the choice of the Grover oracle, since Nahimovs and Santos showed that the loopless coined quantum walk with the Grover oracle also has this exceptional configuration [NS16].

Chapter 5

Analysis of Lackadaisical Quantum Walks on Locally Arc-Transitive Graphs

Our original contribution begins in this chapter, where we analyze the complexity and success probability of lackadaisical quantum walks on locally arc-transitive graphs. Rhodes and Wong [RW20] and the other aforementioned work consider lackadaisical quantum walks on certain instances and classes of regular vertex-transitive graphs. One common property of these instances and classes of graphs is that they are locally arc-transitive. We simulate lackadaisical quantum walks and quantum interpolated walks on locally arc-transitive graphs. From the simulation results shown in Appendix B, we find that the lackadaisical quantum walk is closely related to the quantum interpolated walk.

In this chapter, we establish a relationship between the lackadaisical quantum walk and the quantum interpolated walk on any regular locally arc-transitive graph with a unique marked vertex. This relationship permits us to analyze the quantum hitting time and behaviour of lackadaisical quantum walks, which proves the conjectures and numerical findings in [RW20] and the other earlier work on the complexity and success probability of lackadaisical quantum walks on those graphs.

5.1 A variant of lackadaisical quantum walk

To show the relationship for any d-regular locally arc-transitive graph G with a unique marked vertex m, we introduce a variant of the lackadaisical quantum walk as an intermediate quantum walk operator. The lackadaisical quantum walk A_{lazy} uses a Grover oracle Q as defined in Equation 4.3. We define a different oracle as

$$\widehat{\mathsf{Q}} = \mathsf{I}_{(d+1)N} - 2\big(|m, \circlearrowleft\rangle\langle m, \circlearrowleft| + |m, \oplus\rangle\langle m, \oplus|\big), \tag{5.1}$$

where

$$|\oplus\rangle = \frac{1}{\sqrt{d}} \sum_{k=1}^{d} |e_k\rangle$$

denotes an equally weighted superposition over all the d outgoing arcs of any vertex. Using the query $\widehat{\mathsf{Q}}$, we define the following variant of lackadaisical quantum walks,

$$\widehat{\mathsf{A}}_{lazy} = \mathsf{W}_{lazy} \cdot \widehat{\mathsf{Q}}.$$

We first show that we can replace the oracle Q with the oracle $\widehat{\mathsf{Q}}$ without altering the evolution of the walk. Write the state of the system after t steps of the walk A_{lazy} on the initial state $|\overline{\text{init}}_{lazy}\rangle$,

$$\mathsf{A}_{lazy}^{t}|\overline{\text{init}}_{lazy}\rangle = \Bigg(\sum_{u \neq m;\, k} \alpha_{u,k}|u, e_k\rangle\Bigg) + \Bigg(\sum_{k} \alpha_{m,k}|m, e_k\rangle\Bigg) + \Bigg(\sum_{v \in V(G)} \alpha_{v,\circlearrowleft}|v, \circlearrowleft\rangle\Bigg), \tag{5.2}$$

for some amplitudes α. We show that local arc-transitivity implies that the amplitudes of the outgoing arcs of the marked vertex m remain equal after any number of iterations.

Lemma 25 ([HY20]). *On any d-regular locally arc-transitive graph G with a unique marked vertex m, for all $t \geq 0$, $\alpha_{m,i} = \alpha_{m,j}$ for all outgoing arcs (m, y_j) and (m, y_k) of the marked* *vertex m.*

Proof. We define an application of an automorphism σ of G on quantum states and operators acting on $\mathcal{H}_N \otimes \mathcal{H}_{d+1}$ as follows. For any vertex x and its j^{th} outgoing arc (x, y), let $\sigma(|x, e_j\rangle) = |x', e_k\rangle$, where $\sigma(x) = x'$ and $\sigma(y) = y'$, and (x', y') is the k^{th} arc from x'. For any vertex x and its self-loop, let $\sigma(|x, \circlearrowleft\rangle) = |x', \circlearrowleft\rangle$. Generalize and define the action on the adjoint as $\sigma(\langle x, e_j|) = \langle x', e_k|$ and $\sigma(\langle x, \circlearrowleft|) = \langle x', \circlearrowleft|$, and extend to operators and the entire Hilbert space by composition and linearity.

For any automorphism σ, we thus have $\sigma(\mathsf{S}_{\text{ff}}) = \mathsf{S}_{\text{ff}}$, since S_{ff} changes the direction of every arc. Similarly, $\sigma(\mathsf{I}_N \otimes \mathsf{C}) = (\mathsf{I}_N \otimes \mathsf{C})$, since an automorphism preserves the neighborhood of any vertex.

Let v_1 and v_2 be the endpoints of any two distinct outgoing arcs of m (excluding the self-loop). Since G is locally arc-transitive, there exists an automorphism σ_m that fixes m and that maps the arc (m, v_1) to (m, v_2). Let Δ_m be a set of $d(d-1)$ such automorphisms, one for each pair v_1, v_2 of distinct neighbors of m. For any automorphism $\sigma_m \in \Delta_m$ we have that $\sigma_m(\mathsf{Q}) = \mathsf{Q}$ and $\sigma_m\left(|\overline{\text{init}}_{lazy}\rangle\right) = |\overline{\text{init}}_{lazy}\rangle$.

The proof of the lemma now follows readily by mathematical induction on t. Assume that $\sigma_m\left(\mathsf{A}^t_{lazy}|\overline{\text{init}}_{lazy}\rangle\right) = \mathsf{A}^t_{lazy}|\overline{\text{init}}_{lazy}\rangle$ for any $\sigma_m \in \Delta_m$ immediately prior to the $(t+1)^{\text{th}}$ application of A_{lazy}. Then by the above arguments, it holds immediately after the $(t+1)^{\text{th}}$ application of A_{lazy}. Since $\sigma_m\left(\mathsf{A}^{t+1}_{lazy}|\overline{\text{init}}_{lazy}\rangle\right) = \mathsf{A}^{t+1}_{lazy}|\overline{\text{init}}_{lazy}\rangle$, then $\sigma_m\left(\sum_k \alpha_{m,k}|m, e_k\rangle\right) = \sum_k \alpha_{m,k}|m, e_k\rangle$, and thus $\alpha_{m,j} = \alpha_{m,k}$ for all outgoing arcs (m, y_j) and (m, y_k). □

Lemma 26 ([HY20]). *On any d-regular locally arc-transitive graph G with a unique marked vertex m, for all $t \geq 0$,*

$$\mathsf{A}^t_{lazy}|\overline{\text{init}}_{lazy}\rangle = \widehat{\mathsf{A}}^t_{lazy}|\overline{\text{init}}_{lazy}\rangle.$$

Proof. The difference between A_{lazy} and $\widehat{\mathsf{A}}_{lazy}$ is that A_{lazy} uses a query to the oracle Q in Equation 4.3 and $\widehat{\mathsf{A}}_{lazy}$ uses a different query operator $\widehat{\mathsf{Q}}$ given by Equation 5.1. By

Lemma 25, Equation 5.2 can be written as

$$\mathsf{A}^t_{lazy}|\overline{\text{init}}_{lazy}\rangle = \left(\sum_{u\neq m;\,k} \alpha_{u,k}|u,e_k\rangle\right) + \alpha_{m,\oplus}|m,\oplus\rangle + \left(\sum_{v\in V(G)} \alpha_{v,\circlearrowleft}|v,\circlearrowleft\rangle\right).$$

On such states where the amplitudes of the outgoing arcs of the marked vertex m are equal, Q and $\widehat{\mathsf{Q}}$ act identically. □

5.2 Quantum interpolated lazy walk

We define a quantum interpolated lazy walk as the second intermediate quantum operator. Given a random walk P on the d-regular graph G, define a lazy random walk as

$$\widehat{\mathsf{P}} = \frac{d}{d+\ell}\cdot\mathsf{P} + \frac{\ell}{d+\ell}\cdot\mathsf{I}_N, \tag{5.3}$$

obtained by adding a self-loop of weight ℓ to every vertex. The interpolation of a lazy random walk is then denoted

$$\widehat{\mathsf{P}}(s) = (1-s)\cdot\widehat{\mathsf{P}} + s\cdot\widehat{\mathsf{P}}', \tag{5.4}$$

where $\widehat{\mathsf{P}}' = (\widehat{\mathsf{P}})'$ is the absorbing walk derived from the lazy random walk $\widehat{\mathsf{P}}$. Then we apply Szegedy's correspondence on $\widehat{\mathsf{P}}(s)$ to obtain the quantum interpolated lazy walk $\mathsf{W}(\widehat{\mathsf{P}}(s))$. The initial state of $\mathsf{W}(\widehat{\mathsf{P}}(s))$ is

$$|\overline{\text{init}}_{\hat{ip}}\rangle = \frac{1}{\sqrt{N-|M|}}\sum_{x\notin M}|x\rangle\otimes|\widehat{\mathsf{P}}(s)_x\rangle.$$

For the convenience of comparison, we denote by $|\overline{\text{init}}_{ip}\rangle$ the initial state of the quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$, instead of $|\overline{\text{init}}\rangle$ that we use in Section 3.1.

Consider the two quantum walks $\mathsf{W}(\widehat{\mathsf{P}}(s))$ and $\widehat{\mathsf{A}}_{lazy}$. Recall that in Section 2.3 we use the isometry E to identify the search space of Szegedy's quantum walks with that of coined quantum walks. Similarly, we identify the search space of $\mathsf{W}(\widehat{\mathsf{P}}(s))$ with that of $\widehat{\mathsf{A}}_{lazy}$ by extending the isometry E so that it maps $\mathbb{C}^{(d+1)N}$ to $\mathcal{H}_N \otimes \mathcal{H}_{d+1}$ as follows.

For all vertices x in the graph G, and all k^{th} neighbors y_k of x, define the isometry $\mathsf{E}\colon \mathbb{C}^{(d+1)N} \longrightarrow \mathcal{H}_N \otimes \mathcal{H}_{d+1}$ as follows,

$$\mathsf{E}\colon \begin{cases} |x, y_k\rangle & \mapsto \quad |x, e_k\rangle \\ |x, x\rangle & \mapsto \quad |x, \circlearrowleft\rangle \quad \text{if } x \notin M \text{ is unmarked} \\ |x, x\rangle & \mapsto -|x, \circlearrowleft\rangle \quad \text{if } x \in M \text{ is marked.} \end{cases}$$

Lemma 27 ([HY20]). *Given a d-regular graph G, let $\widehat{\mathsf{A}}_{lazy}$ be a lackadaisical quantum walk with self-loops of weight ℓ and $\mathsf{W}(\widehat{\mathsf{P}}(s))$ be a quantum interpolated lazy walk with $s = 1 - \frac{\ell}{d}$. Then*

$$\widehat{\mathsf{A}}_{lazy} = \mathsf{E} \cdot \mathsf{W}(\widehat{\mathsf{P}}(s)) \cdot \mathsf{E}^{\dagger}.$$

Proof. The quantum circuit of the quantum walk $\widehat{\mathsf{A}}_{lazy} = \mathsf{W}_{lazy} \cdot \widehat{\mathsf{Q}}$ is given in Figure 5.1.

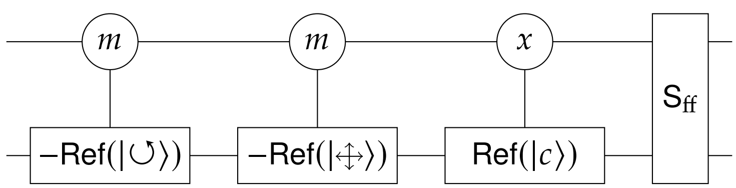

Figure 5.1: Circuit of the quantum walk $\widehat{\mathsf{A}}_{lazy}$.

The two states $|\circlearrowleft\rangle$ and $|\leftrightarrow\rangle$ are orthogonal, and they span a two-dimensional subspace of the coin space $\mathcal{H}_{d+1}$. The coin state $|c\rangle = \sqrt{\frac{d}{d+\ell}}|\leftrightarrow\rangle + \sqrt{\frac{\ell}{d+\ell}}|\circlearrowleft\rangle$ is in this two-dimensional subspace. Let $|c^{\perp}\rangle = \sqrt{\frac{\ell}{d+\ell}}|\leftrightarrow\rangle - \sqrt{\frac{d}{d+\ell}}|\circlearrowleft\rangle$ be the state that is orthogonal to the coin state $|c\rangle$ in this two-dimensional subspace. In Figure 5.1, we apply three reflections on the coin register if the vertex x is marked, and we apply a single reflection if the vertex is unmarked. In either case, we apply an odd number of reflections on the coin register.

We can therefore rewrite the circuit in Figure 5.1 as the equivalently acting circuit given in Figure 5.2.

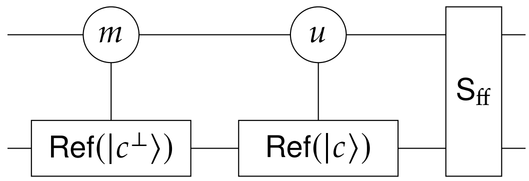

Figure 5.2: Equivalent circuit of $\widehat{\mathsf{A}}_{lazy}$.

For the lazy random walk $\widehat{\mathsf{P}}$ with self-loops of weight ℓ, the neighbourhood state of any vertex x in a regular graph is $|\widehat{\mathsf{P}}_x\rangle = \sqrt{\frac{d}{d+\ell}}|\mathsf{P}_x\rangle + \sqrt{\frac{\ell}{d+\ell}}|x\rangle$. The interpolation of a random walk changes the neighborhood state of any marked vertex. With our choice of $s = 1 - \frac{\ell}{d}$, they become

$$\begin{aligned} |\widehat{\mathsf{P}}(s)_u\rangle &= \sqrt{\tfrac{d}{d+\ell}}|\mathsf{P}_u\rangle + \sqrt{\tfrac{\ell}{d+\ell}}|u\rangle \\ |\widehat{\mathsf{P}}(s)_m\rangle &= \sqrt{\tfrac{\ell}{d+\ell}}|\mathsf{P}_m\rangle + \sqrt{\tfrac{d}{d+\ell}}|m\rangle. \end{aligned}$$

Here u denotes any unmarked vertex, and m denotes any marked vertex. Applying the isometry E yields that

$$\begin{aligned} \mathsf{E}\,|u, \widehat{\mathsf{P}}(s)_u\rangle &= |u, c\rangle \\ \mathsf{E}\,|m, \widehat{\mathsf{P}}(s)_m\rangle &= |m, c^{\perp}\rangle. \end{aligned} \tag{5.5}$$

By definition, the $\mathsf{S_{ff}}$ operator is equivalent to the SWAP operator under the isometry,

$$\mathsf{S_{ff}} = \mathsf{E} \cdot \mathsf{SWAP} \cdot \mathsf{E}^{\dagger}. \tag{5.6}$$

Equations 5.5 and 5.6 permit us to write the coined quantum walk circuit in Figure 5.2 as a circuit of the quantum interpolated walk $\mathsf{E} \cdot \mathsf{W}(\widehat{\mathsf{P}}(s)) \cdot \mathsf{E}^{\dagger}$, as in Figure 5.3. □

When there is a unique marked vertex in the graph, the value of ℓ used in [RW20] is $\ell = \frac{d}{N}$, and the value of ℓ proposed in [WZWY17] is $\ell = \frac{d}{N-1}$. The difference between these two values of ℓ is an additive term of order $\frac{1}{N^2}$. In this work, we pick the value of

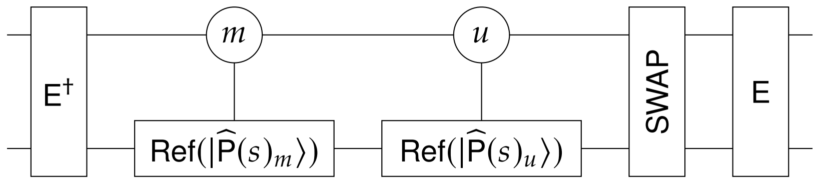

Figure 5.3: $\widehat{\mathsf{A}}_{lazy}$ written as a circuit of $\mathsf{E} \cdot \mathsf{W}(\widehat{\mathsf{P}}(s)) \cdot \mathsf{E}^\dagger$.

ℓ to be equal to $\frac{d}{N}$, so that the correspondence with [RW20] in Lemma 27 is exact. The value of s used in [KMOR16], and in the simulation in Section 7 in [DH17], is $1 - \frac{1}{N-1}$ by Equation 3.16, which corresponds to a value of ℓ equal to $\frac{d}{N-1}$. By Equation 3.6, our slightly different choice of ℓ implies that the $\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s))$ used in our paper is a factor of order $\frac{1}{N}$ larger than the $\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s))$ used in [KMOR16]. This negligible factor does not change the results stated in this thesis.

5.3 Quantum hitting time of A_{lazy}

By Lemma 26, we have

$$\mathsf{QHT}_{\mathrm{cot}}(\mathsf{A}_{lazy}, |\overline{\mathrm{init}}_{lazy}\rangle) = \mathsf{QHT}_{\mathrm{cot}}(\widehat{\mathsf{A}}_{lazy}, |\overline{\mathrm{init}}_{lazy}\rangle),$$

By Lemma 27 and the definition of the isometry E, we have

$$\mathsf{QHT}_{\mathrm{cot}}(\widehat{\mathsf{A}}_{lazy}, |\overline{\mathrm{init}}_{lazy}\rangle) = \mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}(\widehat{\mathsf{P}}(s)), |\overline{\mathrm{init}}_{\hat{ip}}\rangle).$$

We next show the relationship between $\mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}(\widehat{\mathsf{P}}(s)), |\overline{\mathrm{init}}_{\hat{ip}}\rangle)$ and $\mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\mathrm{init}}_{ip}\rangle)$

Lemma 28 ([HY20])**.** *On any d-regular graph G with a unique marked vertex, let $\ell = \frac{d}{N}$ and $s = 1 - \frac{\ell}{d} = 1 - \frac{1}{N}$,*

$$\mathsf{QHT}^2_{\mathrm{cot}}(\mathsf{W}(\widehat{\mathsf{P}}(s)), |\overline{\mathrm{init}}_{\hat{ip}}\rangle) = \frac{N+1}{N}\mathsf{QHT}^2_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\mathrm{init}}_{ip}\rangle) + \frac{1}{2N-1}.$$

Proof. By definitions of $\widehat{\mathsf{P}}$ and $\widehat{\mathsf{P}}(s)$, given by Equations 5.3 and 5.4, respectively,

$$\widehat{\mathsf{P}}(s) = \frac{N}{N+1} \cdot \mathsf{P}(s) + \frac{1}{N+1} \cdot \mathsf{I}_N.$$

Hence $\widehat{\mathsf{P}}(s)$ and $\mathsf{P}(s)$ have the same eigenvectors $|\widehat{\lambda}_k\rangle = |\lambda_k\rangle$ and corresponding eigenvalues

$$\widehat{\lambda}_k = \frac{N}{N+1}\lambda_k + \frac{1}{N+1}. \tag{5.7}$$

Then by definition of the interpolated hitting time in Equation 3.5,

$$\mathsf{HT}_{\text{ip}}(\widehat{\mathsf{P}}(s)) = \frac{N+1}{N} \cdot \mathsf{HT}_{\text{ip}}(\mathsf{P}(s)). \tag{5.8}$$

By Lemma 19, we have

$$\mathsf{QHT}_{\text{cot}}\mathsf{W}(\mathsf{P}(s))|\overline{\text{init}}_{ip}\rangle^2 = 2\mathsf{HT}_{\text{ip}}(\mathsf{P}(s)) - \frac{p_M}{1-s(1-p_M)}, \tag{5.9}$$

where p_M is the probability of drawing a marked vertex from the stationary distribution $\vec{\pi}$. Since our graph is regular and there is a unique marked vertex, $p_M = \pi_m = \frac{1}{N}$. Lemma 28 follows from substituting Equation 5.9 into Equation 5.8 on both sides. □

We now prove that the quantum hitting time of lackadaisical quantum walks is in $O(\sqrt{\mathsf{HT}})$ in Theorem 29.

Theorem 29 ([HY20])**.** *Consider a d-regular locally arc-transitive graph with N vertices and a unique marked vertex m. For the lackadaisical quantum walk A_{lazy}, add self-loops of weight $\ell = \frac{d}{N}$ on every vertex. For the quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$, choose $s = 1 - \frac{\ell}{d}$. Then*

$$\mathsf{QHT}^2_{\text{cot}}(\mathsf{A}_{lazy}, |\overline{\text{init}}_{lazy}\rangle) = \frac{N+1}{N}\mathsf{QHT}^2_{\text{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\text{init}}_{ip}\rangle) + \frac{1}{2N-1},$$

and

$$\mathsf{QHT}_{\mathrm{cot}}(\mathsf{A}_{lazy}, |\overline{\mathrm{init}}_{lazy}\rangle) \in O\Big(\sqrt{\mathsf{HT}(\mathsf{P}, \{m\})}\Big).$$

Proof. Theorem 29 directly follows from Lemmas 26, 27 and 28. The quantum hitting time $\mathsf{QHT}_{\mathrm{cot}}(\mathsf{W}(\mathsf{P}(s)), |\overline{\mathrm{init}}_{ip}\rangle)$ is in $O\big(\sqrt{\mathsf{HT}(\mathsf{P}, \{m\})}\big)$ follows from Lemma 19 and the fact that $\mathsf{HT}_{\mathrm{ip}}(\mathsf{P}(s)) \leq \mathsf{HT}(\mathsf{P}, \{m\})$ when there is a unique marked vertex. □

5.4 Quantum states after applying A_{lazy}

By Lemmas 26 and 27, the quantum states after applying A_{lazy} and $\mathsf{W}(\widehat{\mathsf{P}}(s))$ on the initial states for any steps are identical under the isometry E. In the section, we show the upper bound of the L^2-distance between quantum states after applying $\mathsf{W}(\widehat{\mathsf{P}}(s))$ and $\mathsf{W}(\mathsf{P}(s))$ on the initial states. For convenience, from now on, we will omit the interpolation parameter s when analyzing the spectra of $\mathsf{W}(\mathsf{P}(s))$ and $\mathsf{W}(\widehat{\mathsf{P}}(s))$. We use the notation "$\widehat{\ }$" when referring to the spectra of $\mathsf{W}(\widehat{\mathsf{P}}(s))$.

By the spectral decomposition in Theorem 12, the eigenvectors $|\phi_k^{\pm}\rangle$ of $\mathsf{W}(\mathsf{P}(s))$ are in the subspace

$$\mathrm{span}\big\{\mathsf{T}(s)|\lambda_k\rangle, \mathsf{SWAP}\cdot\mathsf{T}(s)|\lambda_k\rangle\big\} = \mathrm{span}\big\{\mathsf{T}(s)|\lambda_k\rangle, (\mathsf{T}(s)|\lambda_k\rangle)^{\perp}\big\}.$$

Applying Szegedy's correspondence on $\widehat{\mathsf{P}}(s)$ is similar, except we use '$\widehat{\ }$' when referring to $\widehat{\mathsf{P}}(s)$. The eigenvectors $|\widehat{\phi}_k^{\pm}\rangle$ of $\mathsf{W}(\widehat{\mathsf{P}}(s))$ are in the subspace

$$\mathrm{span}\big\{\widehat{\mathsf{T}}(s)|\lambda_k\rangle, \mathsf{SWAP}\cdot\widehat{\mathsf{T}}(s)|\lambda_k\rangle\big\} = \mathrm{span}\big\{\widehat{\mathsf{T}}(s)|\lambda_k\rangle, (\widehat{\mathsf{T}}(s)|\lambda_k\rangle)^{\perp}\big\}.$$

We define an isometry

$$\mathsf{R}_1 = \sum_x \big(|x, \widehat{\mathsf{P}}(s)_x\rangle\langle x, \mathsf{P}(s)_x| + |x, \widehat{\mathsf{P}}(s)_x^{\perp}\rangle\langle x, \mathsf{P}(s)_x^{\perp}|\big),$$

where $|x, \mathsf{P}(s)_x^{\perp}\rangle$ is orthogonal to $|x, \mathsf{P}(s)_x\rangle$ in the subspace spanned by $\{|x, \mathsf{P}(s)_x\rangle, |\mathsf{P}(s)_x, x\rangle\}$ and $|x, \widehat{\mathsf{P}}(s)_x^{\perp}\rangle$ is orthogonal to $|x, \widehat{\mathsf{P}}(s)_x\rangle$ in the subspace spanned by $\{|x, \widehat{\mathsf{P}}(s)_x\rangle, |\widehat{\mathsf{P}}(s)_x, x\rangle\}$. The isometry R_1 satisfies that

$$\mathsf{R}_1 \colon \begin{cases} |\phi_0\rangle & \mapsto \quad |\widehat{\phi}_0\rangle \\ |\phi_k^+\rangle & \mapsto \quad |\widehat{\phi}_k^{\,+}\rangle \\ |\phi_k^-\rangle & \mapsto \quad |\widehat{\phi}_k^{\,-}\rangle. \end{cases}$$

By the decomposition of $|\overline{\mathrm{init}}_{ip}\rangle$ in Equation 3.10, applying the quantum walk $\mathsf{W}(\mathsf{P}(s))$ on the initial state $|\overline{\mathrm{init}}_{ip}\rangle$ for t times yields the state

$$\mathsf{W}(\mathsf{P}(s))^t|\overline{\mathrm{init}}_{ip}\rangle = \alpha_0|\phi_0\rangle + \frac{1}{\sqrt{2}}\sum_{k=1}^{N-1}\alpha_k\big((e^{i\theta_k})^t|\phi_k^+\rangle + (e^{-i\theta_k})^t|\phi_k^-\rangle\big). \tag{5.10}$$

Applying R_1 on the state $\mathsf{W}(\mathsf{P}(s))^t|\overline{\mathrm{init}}_{ip}\rangle$ changes the eigenspace of $\mathsf{W}(\mathsf{P}(s))$ to the eigenspace of $\mathsf{W}(\widehat{\mathsf{P}}(s))$,

$$\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t|\overline{\mathrm{init}}_{ip}\rangle = \alpha_0|\widehat{\phi}_0\rangle + \frac{1}{\sqrt{2}}\sum_{k=1}^{N-1}\alpha_k\big((e^{i\theta_k})^t|\widehat{\phi}_k^{\,+}\rangle + (e^{-i\theta_k})^t|\widehat{\phi}_k^{\,-}\rangle\big).$$

In the proof of Lemma 30 below, we require a second isometry, which is also a projection,

$$\mathsf{R}_2 = \sum_x \big(|x, \mathsf{P}(s)_x\rangle\langle x, \mathsf{P}(s)_x| + |x, \mathsf{P}(s)_x^{\perp}\rangle\langle x, \mathsf{P}(s)_x^{\perp}|\big).$$

Applying R_2 on $\mathsf{W}(\mathsf{P}(s))^t|\overline{\mathrm{init}}_{ip}\rangle$ does not change the state itself,

$$\mathsf{R}_2 \cdot \mathsf{W}(\mathsf{P}(s))^t|\overline{\mathrm{init}}_{ip}\rangle = \mathsf{W}(\mathsf{P}(s))^t|\overline{\mathrm{init}}_{ip}\rangle.$$

Note that since the states $|\mathsf{P}(s)_x\rangle$ and $|\widehat{\mathsf{P}}(s)_x\rangle$ are close for all vertices x, the L^2-distance between R_1 and R_2 is small, which is $O\big(\frac{1}{\sqrt{N}}\big)$ by direct calculation.

Lemma 30 ([HY20]). *For all $t \geq 0$,*

$$\left\|\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle - \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle\right\|_2 \in O\left(\frac{1}{\sqrt{N}}\right).$$

Proof.

$$\begin{aligned}
&\left\|\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle - \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle\right\|_2 \\
&= \left\|\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle - \mathsf{R}_2 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle\right\|_2 \\
&\leq \left\|\mathsf{R}_1 - \mathsf{R}_2\right\|_2 \cdot \left\|\mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle\right\|_2 = \left\|\mathsf{R}_1 - \mathsf{R}_2\right\|_2 \in O\left(\frac{1}{\sqrt{N}}\right).
\end{aligned}$$

□

Next, consider the following L^2-distance

$$\begin{aligned}
&\left\|\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle - \mathsf{W}(\widehat{\mathsf{P}}(s))^t \cdot |\overline{\mathrm{init}}_{i\hat{p}}\rangle\right\|_2 \\
&= \left\|\frac{1}{\sqrt{2}} \sum_{k=1}^{N-1} \alpha_k \Big((e^{ti\theta_k} - e^{ti\widehat{\theta}_k})|\widehat{\phi}_k^+\rangle + (e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k})|\widehat{\phi}_k^-\rangle\Big)\right\|_2.
\end{aligned}$$

We pick a threshold angle θ_0 satisfying $0 < \theta_0 \leq \frac{\pi}{2}$ and separate the sum into two parts, where the first part is for angles $0 < \theta_k \leq \theta_0$ and the second part is for $\theta_0 < \theta_k \leq \pi$. We give an upper bound on the L^2-norm for each of these two parts in Facts 31 and 32, respectively.

Fact 31 ([HY20]). *For $0 < \theta_0 \leq \frac{\pi}{2}$ and all $t \geq 0$,*

$$\left\|\frac{1}{\sqrt{2}} \sum_{0<\theta_k\leq\theta_0} \alpha_k \Big((e^{ti\theta_k} - e^{ti\widehat{\theta}_k})|\widehat{\phi}_k^+\rangle + (e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k})|\widehat{\phi}_k^-\rangle\Big)\right\|_2 \leq \frac{8t}{N-1} \sin\left(\frac{\theta_0}{2}\right).$$

Proof.

$$
\begin{aligned}
&\left\| \frac{1}{\sqrt{2}} \sum_{0<\theta_k \leq \theta_0} \alpha_k \Big((e^{ti\theta_k} - e^{ti\widehat{\theta}_k}) |\widehat{\phi}_k^{\,+}\rangle + (e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k}) |\widehat{\phi}_k^{\,-}\rangle \Big) \right\|_2 \\
&= \frac{1}{\sqrt{2}} \sqrt{\sum_{0<\theta_k \leq \theta_0} |\alpha_k|^2 \Big(|e^{ti\theta_k} - e^{ti\widehat{\theta}_k}|^2 + |e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k}|^2 \Big)} \\
&\leq \max_{\theta_k \leq \theta_0} \left| e^{ti\theta_k} - e^{ti\widehat{\theta}_k} \right| \sqrt{\sum_{0<\theta_k \leq \theta_0} |\alpha_k|^2} \\
&\leq \max_{\theta_k \leq \theta_0} \left| e^{ti\theta_k} - e^{ti\widehat{\theta}_k} \right| \\
&= \max_{\theta_k \leq \theta_0} \left| 2 \sin\left(t \frac{\theta_k - \widehat{\theta}_k}{2} \right) \right| \\
&= \max_{\theta_k \leq \theta_0} \left| 2 \sin\left(\frac{2t}{N+1} \frac{N+1}{2} \frac{\theta_k - \widehat{\theta}_k}{2} \right) \right| \\
&\leq \frac{8t}{N-1} \sin\left(\frac{\theta_0}{2} \right).
\end{aligned}
$$

In the last inequality, by Equation 5.7, since $0 < \theta_k \leq \theta_0 \leq \frac{\pi}{2}$, then $(1 - \frac{2}{N+1})\theta_k \leq \widehat{\theta}_k \leq \theta_k$, which implies that $0 \leq \frac{N+1}{2} \frac{\theta_k - \widehat{\theta}_k}{2} \leq \frac{\theta_0}{2}$. Finally $\sin(ax) \leq 2a \sin(x)$ for all $0 \leq x \leq \pi/4$ and all $a \geq 0$. ◻

Fact 32 ([HY20]). *For $0 < \theta_0 \leq \frac{\pi}{2}$ and all $t \geq 0$,*

$$
\left\| \frac{1}{\sqrt{2}} \sum_{\theta_0<\theta_k \leq \pi} \alpha_k \Big((e^{ti\theta_k} - e^{ti\widehat{\theta}_k}) |\widehat{\phi}_k^{\,+}\rangle + (e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k}) |\widehat{\phi}_k^{\,-}\rangle \Big) \right\|_2 \leq \frac{2}{\sqrt{(1-\cos\theta_0)(N-1)}}.
$$

Proof. First, simplify by bounding each factor $\left| e^{ti\theta_k} - e^{ti\widehat{\theta}_k} \right|$ by its trivial upper bound of 2,

$$
\begin{aligned}
&\left\| \frac{1}{\sqrt{2}} \sum_{\theta_0<\theta_k \leq \pi} \alpha_k \Big((e^{ti\theta_k} - e^{ti\widehat{\theta}_k}) |\widehat{\phi}_k^{\,+}\rangle + (e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k}) |\widehat{\phi}_k^{\,-}\rangle \Big) \right\|_2 \\
&\leq \max_{\theta_0<\theta_k} \left| e^{ti\theta_k} - e^{ti\widehat{\theta}_k} \right| \sqrt{\sum_{\theta_0<\theta_k \leq \pi} |\alpha_k|^2} \leq 2 \sqrt{\sum_{\theta_0<\theta_k \leq \pi} |\alpha_k|^2}.
\end{aligned}
$$

We next upper bound the sum of the scalars α_k^2 for the large angles $\theta_0 < \theta_k \leq \pi$ by $\frac{1}{(1-\cos\theta_0)(N-1)}$. For this, consider the quantum walk $\mathsf{W}(\mathsf{P}(s))$,

$$\langle\overline{\text{init}}_{ip}|\mathsf{W}(\mathsf{P}(s))|\overline{\text{init}}_{ip}\rangle = \langle U|\mathsf{D}(\mathsf{P}(s))|U\rangle = 1 - \frac{1}{N-1}.$$

By Equation 3.9, we have

$$\langle U|\mathsf{D}(\mathsf{P}(s))|U\rangle = \sum_{k=0}^{N-1} \lambda_k \alpha_k^2.$$

Using the fact that $\sum_{k=0}^{N-1} \alpha_k^2 = 1$, we infer that

$$\begin{aligned} 1 - \langle U|\mathsf{D}(\mathsf{P}(s))|U\rangle &= \sum_{k=0}^{N-1} \alpha_k^2 - \sum_{k=0}^{N-1} \lambda_k \alpha_k^2 = \sum_{k=0}^{N-1} (1-\lambda_k)\alpha_k^2 \\ &= \sum_{0<\theta_k\leq\theta_0} (1-\lambda_k)\alpha_k^2 + \sum_{\theta_0<\theta_k\leq\pi} (1-\lambda_k)\alpha_k^2 \\ &= \frac{1}{N-1}. \end{aligned}$$

Since $-1 \leq \lambda_k \leq 1$ for all k, we have $\sum_{0<\theta_k\leq\theta_0}(1-\lambda_k)\alpha_k^2 \geq 0$. For $\theta_0 < \theta_k \leq \pi$, i.e. $\lambda_k < \cos\theta_0$, we conclude that

$$\sum_{\theta_0<\theta_k\leq\pi} \alpha_k^2 \leq \frac{1}{1-\cos\theta_0} \sum_{\theta_0<\theta_k\leq\pi} (1-\lambda_k)\alpha_k^2 \leq \frac{1}{(1-\cos\theta_0)(N-1)}.$$

□

Lemma 33 ([HY20]). *Fix a constant $c \geq 1$, then for all $t \leq c\sqrt{\mathsf{HT}(\mathsf{P}, \{m\})}$,*

$$\left\|\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\text{init}}_{ip}\rangle - \mathsf{W}(\widehat{\mathsf{P}}(s))^t \cdot |\overline{\text{init}}_{\hat{ip}}\rangle\right\|_2 \in O\left(\frac{1}{N^{1/4}}\right).$$

Proof. Choose the threshold angle θ_0 such that $\cos\theta_0 = 1 - 2\sqrt{\frac{N-1}{16\mathsf{HT}(\mathsf{P},\{m\})}}$. Since the hitting time $\mathsf{HT}(\mathsf{P}, \{m\})$ for a connected regular graph is at least $N-1$, the threshold angle is well-defined and satisfies that $0 < \theta_0 \le \pi/2$, and thus $0 \le \cos\theta_0 < 1$.

Apply the triangle inequality on Facts 31 and 32, and substitute $\sin\left(\frac{\theta_0}{2}\right) = \left(\frac{N-1}{16\mathsf{HT}(\mathsf{P},\{m\})}\right)^{1/4}$.

$$
\begin{aligned}
&\left\|\mathsf{R}_1 \cdot \mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle - \mathsf{W}(\widehat{\mathsf{P}}(s))^t \cdot |\overline{\mathrm{init}}_{\hat{ip}}\rangle\right\|_2 \\
&= \left\|\frac{1}{\sqrt{2}} \sum_{0<\theta_k\le\pi} \alpha_k \Big((e^{ti\theta_k} - e^{ti\widehat{\theta}_k})|\widehat{\phi}_k^{+}\rangle + (e^{-ti\theta_k} - e^{-ti\widehat{\theta}_k})|\widehat{\phi}_k^{-}\rangle\Big)\right\|_2 \\
&\le \frac{8t}{N-1}\sin\left(\frac{\theta_0}{2}\right) + \frac{2}{\sqrt{(1-\cos\theta_0)(N-1)}} \\
&= \frac{8t}{N-1}\left(\frac{N-1}{16\mathsf{HT}(\mathsf{P},\{m\})}\right)^{1/4} + \frac{\sqrt{2}}{\sqrt{N-1}}\left(\frac{16\mathsf{HT}(\mathsf{P},\{m\})}{N-1}\right)^{1/4} \\
&\le \frac{1}{(N-1)^{3/4}}\left(\frac{8t}{(16\mathsf{HT}(\mathsf{P},\{m\}))^{1/4}} + \sqrt{2}(16\mathsf{HT}(\mathsf{P},\{m\}))^{1/4}\right) \\
&\le \frac{\mathsf{HT}(\mathsf{P},\{m\})^{1/4}}{(N-1)^{3/4}}(4c + 2\sqrt{2}) \\
&\le \frac{2^{1/4}\sqrt{N}}{(N-1)^{3/4}}(4c + 2\sqrt{2}) \\
&\le 9c\frac{\sqrt{N}}{(N-1)^{3/4}} \\
&\in O\left(\frac{1}{N^{1/4}}\right).
\end{aligned}
$$

In the second-last inequality, we apply the upper bound on the hitting time of random walks on regular graphs given in [Fei96], which shows that $\mathsf{HT}(\mathsf{P},\{m\}) \le 2N^2$. □

Lemma 34 ([HY20]). *Fix a constant $c \ge 1$, then for all $t \le c\sqrt{\mathsf{HT}(\mathsf{P},\{m\})}$,*

$$
\left\|\mathsf{W}(\mathsf{P}(s))^t \cdot |\overline{\mathrm{init}}_{ip}\rangle - \mathsf{W}(\widehat{\mathsf{P}}(s))^t \cdot |\overline{\mathrm{init}}_{\hat{ip}}\rangle\right\|_2 \in O\left(\frac{1}{N^{1/4}}\right).
$$

Proof. The result follows by applying the triangle inequality on Lemmas 30 and 33. □

We now prove that L^2-distance between the two quantum states of the lackadaisical quantum walk and the quantum interpolated walk, respectively, remains negligible for any number of steps that is in the order of the quantum hitting time in Theorem 35.

Theorem 35 ([HY20]). *Set* $T_0 = \left\lfloor c \cdot \sqrt{\mathsf{HT}(\mathsf{P}, \{m\})} \right\rfloor$ *for any fixed constant* $c \geq 1$*. For all* $t \leq T_0$*,*

$$\left\| \mathsf{A}_{lazy}^t |\overline{\text{init}}_{lazy}\rangle - \mathsf{E} \cdot \mathsf{W}(\mathsf{P}(s))^t |\overline{\text{init}}_{ip}\rangle \right\|_2 \in O\left(\frac{1}{N^{1/4}}\right).$$

Proof. Theorem 35 follows from Lemmas 27 and 34. □

5.5 Complexity of the lackadaisical quantum walk

From the previous two sections, we prove that the lackadaisical quantum walk A_{lazy} searches regular locally arc-transitive graphs for a unique marked vertex in $O(\sqrt{\mathsf{HT}})$ steps with constant success probability.

Theorem 36 ([HY20]). *Let* G *be a* d*-regular locally arc-transitive graph with* N *vertices and a unique marked vertex* m*, the lackadaisical quantum walk* A_{lazy} *with self-loops of weight* $\ell = \frac{d}{N}$ *finds the marked vertex* m *with constant success probability and complexity of order* $\mathsf{S} + \sqrt{\mathsf{HT}(\mathsf{P}, \{m\})}(\mathsf{C} + \mathsf{U})$.

Chapter 6

Closing Remarks

6.1 Summary of original contributions

In this work, we analytically prove that the lackadaisical quantum walk finds a unique marked vertex with probability at least a constant on any d-regular locally arc-transitive graph when adding self-loops of weight $\ell = \frac{d}{N}$.

The main technical contribution in our work is the use of local arc-transitivity to establish a connection between lackadaisical quantum walks and quantum interpolated walks. We introduce two intermediate quantum walks $\widehat{\mathsf{A}}_{lazy}$ and $\mathsf{W}(\widehat{\mathsf{P}}(s))$ to relate the lackadaisical quantum walks A_{lazy} and the quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$. We show that A_{lazy} acts identically as $\widehat{\mathsf{A}}_{lazy}$ on regular locally arc-transitive graphs with a unique marked vertex. We next prove that $\widehat{\mathsf{A}}_{lazy}$ is equivalent to $\mathsf{W}(\widehat{\mathsf{P}}(s))$ under an isometry and the weight of self-loops ℓ corresponds to an interpolation parameter $s = 1 - \frac{\ell}{d}$ by simplifying the quantum circuit of $\widehat{\mathsf{A}}_{lazy}$. Note that the equivalence between $\widehat{\mathsf{A}}_{lazy}$ and $\mathsf{W}(\widehat{\mathsf{P}}(s))$ does not require the properties of local arc-transitivity and a unique marked vertex. We then construct isometries and use them to upper bound the L^2-distance between the resulting states of $\mathsf{W}(\widehat{\mathsf{P}}(s))$ and $\mathsf{W}(\mathsf{P}(s))$ after any number of steps in the order of the quantum hitting time. We also give an exact relationship between the quantum hitting times of $\mathsf{W}(\widehat{\mathsf{P}}(s))$

and $\mathsf{W}(\mathsf{P}(s))$. Combining the connection that we establish and the analysis of the quantum interpolated walk $\mathsf{W}(\mathsf{P}(s))$ in [KMOR16, DH17], we complete the analytical proof of the complexity and success probability of lackadaisical quantum walks A_{lazy} on regular locally arc-transitive graphs.

Our results prove several speculations and numerical findings in previous work, including the conjectures that lackadaisical quantum walks can find a unique marked vertex in $O(\sqrt{\mathsf{HT}})$ steps with constant success probability on the cycle [GK20], n-dimensional torus [Won18b, WZWY17, RW20], Paley graphs, some Latin square graphs, Johnson graphs, and the hypercube [RW20].

6.2 Future work

We identify the following possible directions to continue our work in this thesis.

The first direction would be considering other types of graphs. The equivalence between the lackadaisical quantum walk A_{lazy} and its variant $\widehat{\mathsf{A}}_{lazy}$ in Lemma 26 depends on the property of local arc-transitivity. For other types of graphs, an approximated relationship may be obtained by bounding the variation between the amplitudes of the neighbours of the marked vertex after each iteration of the walk. One could also introduce different variants by defining oracles other than $\widehat{\mathsf{Q}}$ in Equation 5.1.

Secondly, our results prove that the success probability of lackadaisical quantum walks on regular arc-transitive graphs is at least a constant, and it is interesting to show that the success probability is close to 1. Since we establish a connection between lackadaisical quantum walks and quantum interpolated walks, the spectra of quantum interpolated walks in Theorem 12 may be useful to analyze the success probability. The analysis may depend on the finer structure of different classes of graphs.

Bibliography

[AAKV01] Dorit Aharonov, Andris Ambainis, Julia Kempe, and Umesh Vazirani. Quantum walks on graphs. In *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, STOC'01, pages 50–59, 2001. arXiv:quant-ph/0012090, doi:10.1145/380752.380758.

[ABN+01] Andris Ambainis, Eric Bach, Ashwin Nayak, Ashvin Vishwanath, and John Watrous. One-dimensional quantum walks. In *Proceedings of the 33rd Annual ACM Symposium on Theory of Computing*, STOC'01, pages 37–49, 2001. doi:10.1145/380752.380757.

[AK15] Andris Ambainis and Mārtiņš Kokainis. Analysis of the extended hitting time and its properties, 2015. Poster presented at the 18th Annual Conference on Quantum Information Processing, QIP'15, Sydney, Australia. URL: http://www.quantum-lab.org/qip2015/posters/2-Ambainis.pdf.

[AKR05] Andris Ambainis, Julia Kempe, and Alexander Rivosh. Coins make quantum walks faster. In *Proceedings of the 16th Annual ACM-SIAM Symposium on Discrete Algorithms*, SODA'05, pages 1099–1108, 2005. URL: http://dl.acm.org/citation.cfm?id=1070432.1070590, arXiv:quant-ph/0402107.

[Amb04] Andris Ambainis. Quantum walk algorithm for element distinctness. In *Proceedings of the 45th IEEE Symposium on Foundations of Computer Science*, FOCS'04, pages 22–31, 2004. arXiv:quant-ph/0311001, doi:10.1109/FOCS.2004.54.

[BCWdW01] Harry Buhrman, Richard Cleve, John Watrous, and Ronald de Wolf. Quantum fingerprinting. *Physical Review Letters*, 87(16):167902, 2001. arXiv:quant-ph/0102001, doi:10.1103/PhysRevLett.87.167902.

[BHMT02] Gilles Brassard, Peter Høyer, Michele Mosca, and Alain Tapp. Quantum amplitude amplification and estimation. In *Quantum Computation and Information*, volume 305 of *AMS Contemporary Mathematics*, pages 53–74. American Mathematical Society, 2002. arXiv:quant-ph/0005055.

[CEMM98] Richard Cleve, Artur Ekert, Chiara Macchiavello, and Michele Mosca. Quantum algorithms revisited. *Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences*, 454(1969):339–354, 1998. arXiv:quant-ph/9708016, doi:10.1098/rspa.1998.0164.

[DH17] Cătălin Dohotaru and Peter Høyer. Controlled quantum amplification. In *Proceedings of the 44th International Colloquium on Automata, Languages, and Programming*, volume 80 of *ICALP'17*, pages 18:1–18:13, Dagstuhl, Germany, July 2017. Schloss Dagstuhl–Leibniz-Zentrum für Informatik. doi:10.4230/LIPIcs.ICALP.2017.18.

[Fei96] Uriel Feige. Collecting coupons on trees, and the cover time of random walks. *Computational Complexity*, 6:341–356, 1996. doi:10.1007/BF01270386.

[Fol67] Jon Folkman. Regular line-symmetric graphs. *Journal of Combinatorial Theory*, 3(3):215–232, 1967. doi:10.1016/S0021-9800(67)80069-3.

[Fro12] Ferdinand Georg Frobenius. Über Matrizen aus nicht negativen Elementen. *Sitzungsberichte der Königlich Preussischen Akademie der Wissenschaften*, pages 456–477, May 1912.

[GK20] Pulak Ranjan Giri and Vladimir Korepin. Lackadaisical quantum walk for spatial search. *Modern Physics Letters A*, 35(8):2050043, March 2020. arXiv:1811.06169, doi:10.1142/S0217732320500431.

[Gro96] Lov K. Grover. A fast quantum mechanical algorithm for database search. In *Proceedings of the 28th Annual ACM Symposium on Theory of Computing*, STOC'96, pages 212–219, 1996. arXiv:quant-ph/9605043, doi:10.1145/237814.237866.

[Hol81] Derek F. Holt. A graph which is edge transitive but not arc transitive. *Journal of Graph Theory*, 5(2):201–204, 1981. doi:https://doi.org/10.1002/jgt.3190050210.

[HY20] Peter Høyer and Zhan Yu. Analysis of lackadaisical quantum walks. *Quantum Information & Computation*, 20(13–14):1138–1153, November 2020. arXiv:2002.11234, doi:10.26421/QIC20.13-14.

[Kit95] Alexei Y. Kitaev. Quantum measurements and the Abelian stabilizer problem, 1995. arXiv:quant-ph/9511026.

[KMOR16] Hari Krovi, Frédéric Magniez, Māris Ozols, and Jérémie Roland. Quantum walks can find a marked element on any graph. *Algorithmica*, 74(2):851–907, 2016. arXiv:1002.2419, doi:10.1007/s00453-015-9979-8.

[Mey10] Carl D. Meyer. *Matrix analysis and applied linear algebra*. Society for Industrial and Applied Mathematics, 2010.

[MNRS12] Frédéric Magniez, Ashwin Nayak, Peter C. Richter, and Miklos Santha. On the hitting times of quantum versus random walks. *Algorithmica*, 63(1):91–116, 2012. arXiv:0808.0084, doi:10.1007/s00453-011-9521-6.

[MSS07] Frédéric Magniez, Miklos Santha, and Mario Szegedy. Quantum algorithms for the triangle problem. *SIAM Journal on Computing*, 37(2):413–424, 2007. arXiv:quant-ph/0310134, doi:10.1137/050643684.

[Nah19] Nikolajs Nahimovs. Lackadaisical quantum walks with multiple marked vertices. In *Proceedings of the 45th International Conference on Current Trends in Theory and Practice of Computer Science*, pages 368–378, January 2019. arXiv:1808.00672, doi:10.1007/978-3-030-10801-4_29.

[NC00] Michael Nielsen and Isaac L. Chuang. *Quantum Computation and Information*. Cambridge University Press, 2000.

[NS16] Nikolajs Nahimovs and Raqueline A. M. Santos. *Adjacent vertices can be hard to find by quantum walks*, volume 10139 of *Lecture Notes in Computer Science*, pages 256–267. Springer Berlin Heidelberg, 2016. arXiv:1605.05598, doi:10.1007/978-3-319-51963-0_20.

[Per07] Oskar Perron. Zur Theorie der Matrices. *Mathematische Annalen*, 64(2):248–263, 1907.

[RW19] Mason L. Rhodes and Thomas G. Wong. Search by lackadaisical quantum walks with nonhomogeneous weights. *Physical Review A: General Physics*, 100(4):042303, October 2019. doi:10.1103/PhysRevA.100.042303.

[RW20] Mason L. Rhodes and Thomas G. Wong. Search on vertex-transitive graphs by lackadaisical quantum walk. *Quantum Information Processing*, 19(9), September 2020. arXiv:2002.11227, doi:10.1007/s11128-020-02841-z.

[SKW03] Neil Shenvi, Julia Kempe, and Birgitta K. Whaley. Quantum random-walk search algorithm. *Physical Review A: General Physics*, 67(5):052307, 2003. `arXiv:quant-ph/0210064`, `doi:10.1103/PhysRevA.67.052307`.

[Sze04] Mario Szegedy. Quantum speed-up of Markov chain based algorithms. In *Proceedings of the 45th IEEE Symposium on Foundations of Computer Science*, FOCS'04, pages 32–41, 2004. `doi:10.1109/FOCS.2004.53`.

[Won15] Thomas G. Wong. Grover search with lackadaisical quantum walks. *Journal of Physics A: Mathematical and Theoretical*, 48(43):435304, October 2015. `doi:10.1088/1751-8113/48/43/435304`.

[Won17] Thomas G. Wong. Coined quantum walks on weighted graphs. *Journal of Physics A: Mathematical and Theoretical*, 50(47), October 2017. `doi:10.1088/1751-8121/aa8c17`.

[Won18a] Thomas G. Wong. Corrigendum: Grover search with lackadaisical quantum walks. *Journal of Physics A: Mathematical and Theoretical*, 51(6), January 2018. `doi:10.1088/1751-8121/aa8f54`.

[Won18b] Thomas G. Wong. Faster search by lackadaisical quantum walk. *Quantum Information Processing*, 17(3):68, February 2018. `arXiv:1706.06939`, `doi:10.1007/s11128-018-1840-y`.

[WZWY17] Huiquan Wang, Jie Zhou, Junjie Wu, and Xun Yi. Adjustable self-loop on discrete-time quantum walk and its application in spatial search, July 2017. `arXiv:1707.00601`.

Appendix A

On Local Arc-Transitivity

The main property that we have used in this thesis is local arc-transitivity. The graphs considered in [Won15, Won17, WZWY17, Won18b, RW19, GK20, RW20] are all locally arc-transitive, as well as vertex-transitive, which implies that these graphs are also arc-transitive. The relationship between different graph families is illustrated in Figure A.1.

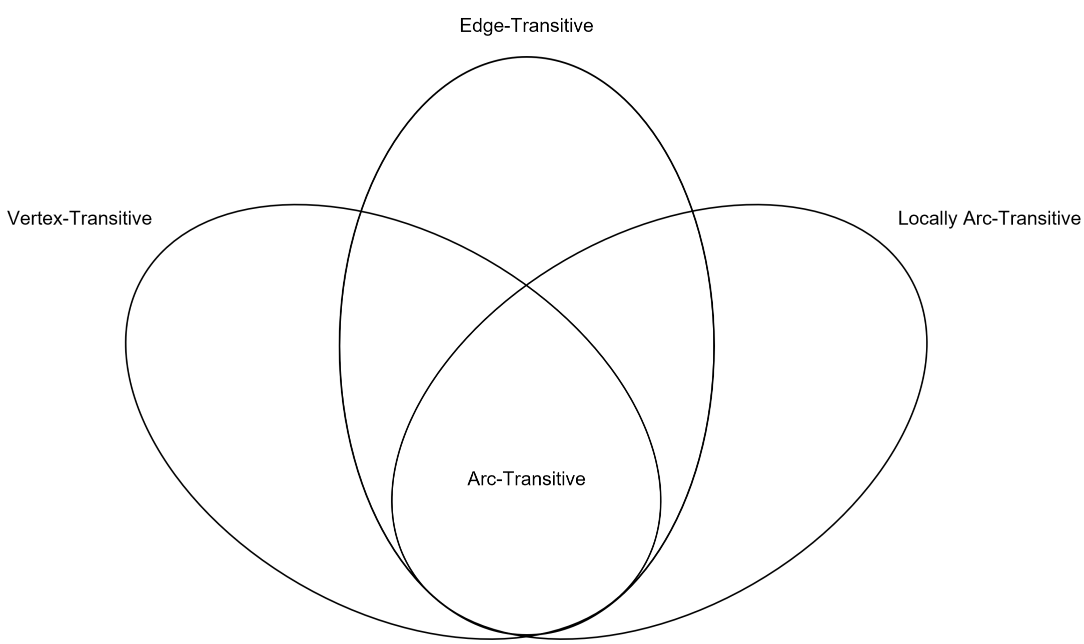

Figure A.1: A Venn Diagram illustrating the relationship between graph families.

We can show that a graph G is arc-transitive if and only if it is locally arc-transitive and vertex-transitive. Trivially, if a graph is arc-transitive, it satisfies the latter conditions. Now, consider the converse. Let (x_1, y_1) and (x_2, y_2) be two arcs in G. Using vertex-transitivity, let σ_1 be an automorphism that maps x_1 to u, and let σ_2 be an automorphism that maps x_2 to u. Using locally arc-transitivity at u, let σ_3 be an automorphism that maps u to u, and that maps $\sigma_1(y_1)$ to $\sigma_2(y_2)$. Then $\sigma_2^{-1}\sigma_3\sigma_1$ maps (x_1, y_1) to (x_2, y_2), and thus G is arc-transitive.

Local arc-transitivity and vertex-transitivity are two distinct graph properties, even when restricting to regular graphs. There are regular graphs that are locally arc-transitive but not vertex-transitive, such as the Folkman graph [Fol67] in Figure A.2. Conversely, there are regular graphs that are vertex-transitive but not locally arc-transitive, such as the Holt graph [Hol81] in Figure A.3. Our analysis in this thesis only applies to regular locally arc-transitive graphs.

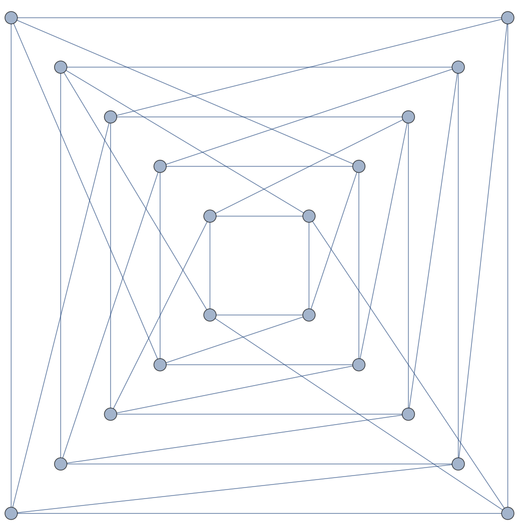

Figure A.2: The Folkman graph.

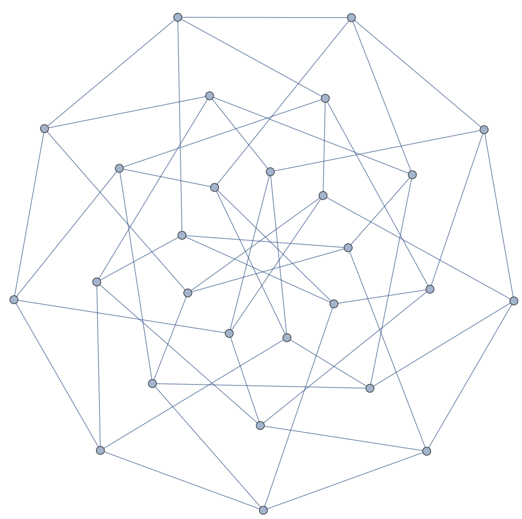

Figure A.3: The Holt graph.

Appendix B

Examples of MATLAB Simulation

We use MATLAB to simulate lackadaisical quantum walks A_{lazy} with self-loops of weight $\ell = \frac{d}{N}$ and quantum interpolated walks $\mathsf{W}(\mathsf{P}(s))$ with $s = 1 - \frac{\ell}{d}$ on a cycle, a 2-dimensional torus, a 3-dimensional torus, a complete graph and a hypercube. The results are shown in the following figures. We observe that the success probability of A_{lazy} and $\mathsf{W}(\mathsf{P}(s))$ are close on those graphs.

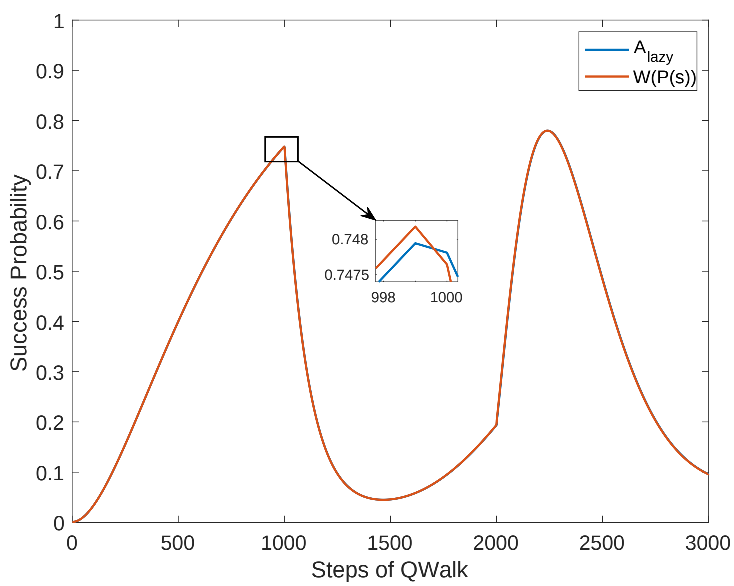

Figure B.1: Two quantum walks on a cycle with $N = 1000$ vertices.

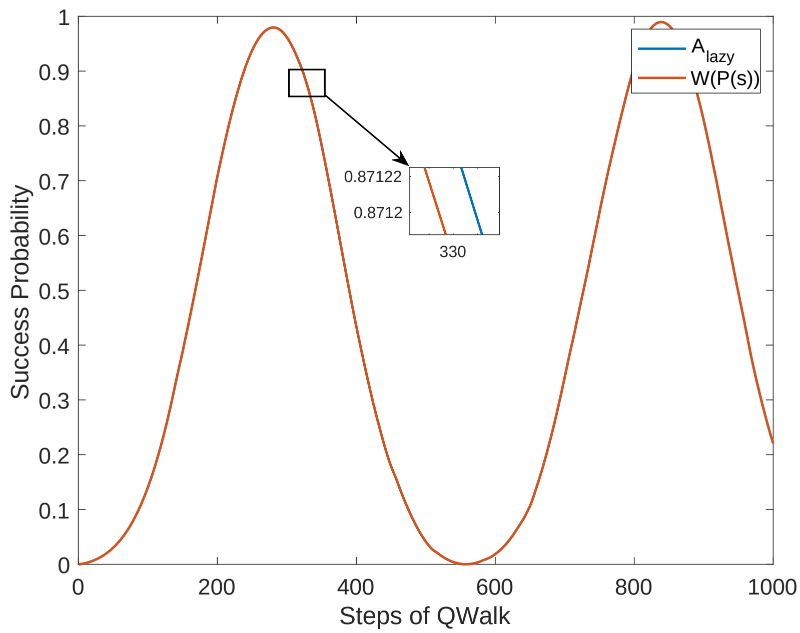

Figure B.2: Two quantum walks on a 2-dimensional 100×100 torus.

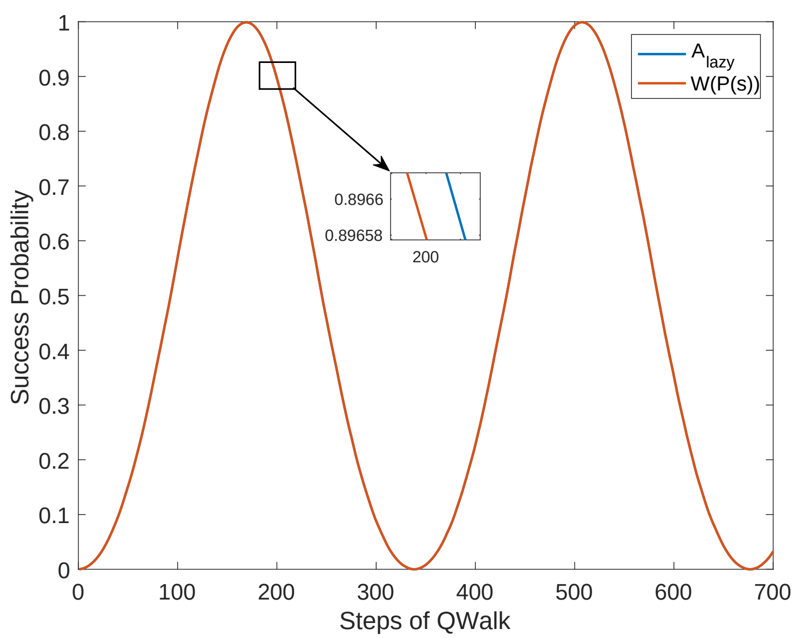

Figure B.3: Two quantum walks on a 3-dimensional $20 \times 20 \times 20$ torus.

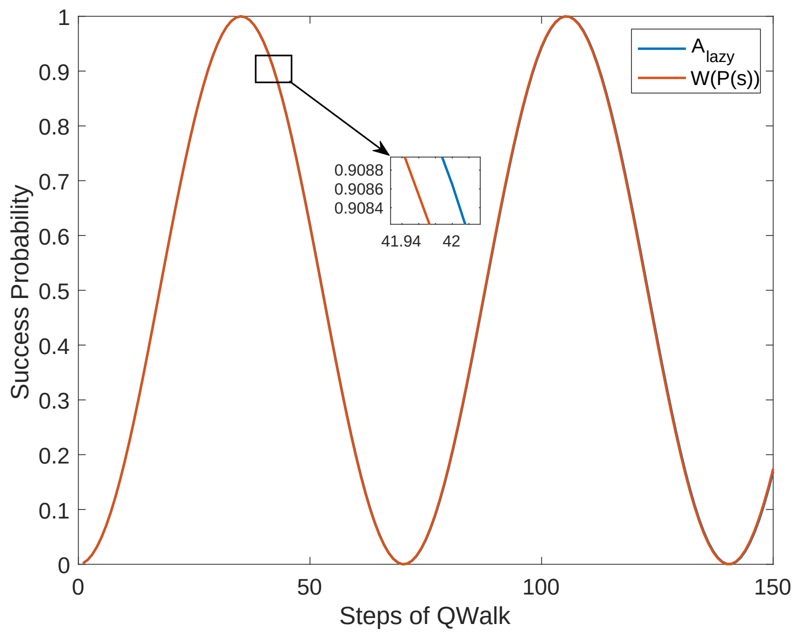

Figure B.4: Two quantum walks on a complete graph with $N = 500$ vertices.

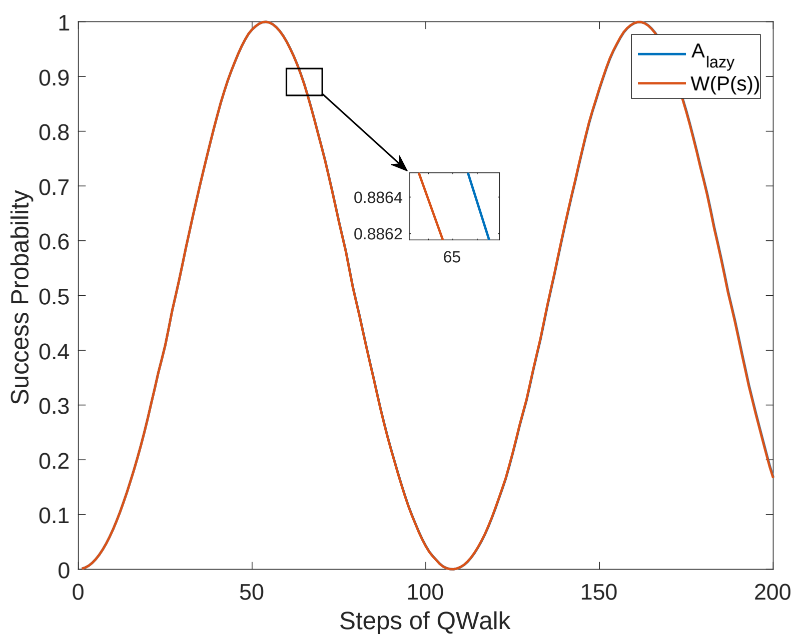

Figure B.5: Two quantum walks on a 10-dimensional hypercube with $N = 2^{10}$ vertices.