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BOSTON UNIVERSITY
GRADUATE SCHOOL OF ARTS AND SCIENCES

Dissertation

ABSORPTION PHENOMENA IN QUANTUM WALKS

by

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B.S., University of Rhode Island, 2013
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ABSORPTION PHENOMENA IN QUANTUM WALKS

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ABSTRACT

The quantum walk is a unitary analogue to the discrete random walk, and its properties have been increasingly studied since the turn of the millenium. In comparison with the classical random walk, the quantum walk exhibits linear spreading and initial condition dependent asymmetries. As noted early on in the conjecture and subsequent calculation of absorption probabilities in the one dimensional Hadamard walk, the interaction of the quantum walk with an absorbing boundary is fundamentally divergent from classical case. Here, we will survey absorption probabilities for a more general collection of one dimensional quantum walks and extend the method to consider d -dimensional walks in the presence of $d - 1$ -dimensional absorbing walls. However, these results are concerned only with local behavior at the boundary in the form of absorption probabilities. The main results of this thesis are concerned with the global behavior of finite quantum walks, which can be described by linear spreading in the short term, modal phenomena in the mid term, and stable distributions in the exceedingly long term. These theorems will be rigorously proved in the one-dimensional case and extrapolated to higher dimensional quantum walks. To this end we introduce `QWSim`, a new and robust computational engine for displaying finite two dimensional quantum walks.

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List of Symbols

\mathbb{Z}	the set of integers
T_x	translation operator
$\ell^2(\mathbb{Z})$	set of square summable functions on the integers
(G, \cdot)	a group under the operation \cdot
Σ	a subset of G
U	a general unitary matrix
$Q \leftrightarrow (G, \Sigma, U)$	quantum walk operator
H	the Hadamard matrix
G_n	the $n \times n$ Grover matrix
C_d	the set of cardinal directions in \mathbb{Z}^d
\tilde{C}_d	the set $C_d \cup \{0\}$
Ψ	a quantum mechanical state
$\Pi_{\text{yes/no}}$	quantum measurement operator

Chapter 1

Introduction

The quantum walk is a quantum mechanical (unitary) analogue of the classical random walk. The proper way to form an analogy between the classical and quantum walks on the integers \mathbb{Z} is to focus on time evolution the probability distribution $f(x)$ of the quantum walker (particle). We define the random walk operator as follows:

Definition 1.1 *Let $T_z : \ell^1(\mathbb{Z}) \rightarrow \ell^1(\mathbb{Z})$ be a translation operator which acts as $(T_z f)(x) = f(x - z)$, and let $0 < p < 1$ with $q = 1 - p$. Then we define the random walk operator $R : \ell^1(\mathbb{Z}) \rightarrow \ell^1(\mathbb{Z})$ as follows:*

$$R = pT_1 + qT_{-1}. \tag{1.1}$$

Note this is an isometry of $\ell^1(\mathbb{Z})$. To construct a quantum mechanical analogue of the classical random walk, we combine properties of this classical random walk transition operator and properties that we expect of a quantum mechanical transition operator. We note that the random walk transition operator (1) acts on functions defined on \mathbb{Z} and (2) is a finite linear combination of translations. From basic postulates of quantum mechanics, we expect a quantum mechanical transition operator Q to (3) act on $L^2(\Omega)$ for some underlying space Ω , and also (4) to be unitary. Choosing $\Omega = \mathbb{Z}$, the question is now whether can we construct an operator $Q : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$ that is unitary and is a finite linear combination of translations? This question is answered in the following lemma (Meyer [50]):

Lemma 1.1 (No-Go Lemma) *The only operator $Q : \ell^2(\mathbb{Z}) \rightarrow \ell^2(\mathbb{Z})$ that is unitary and*

a is finite linear combination of translations is the translation operator up to a phase, i.e. $Q = e^{i\theta}T_z$.

To find an operator Q with nontrivial behavior, we must amend one of the above conditions. This can be done by attaching an additional degree of freedom, a spin with two states R and L , to the underlying space of the quantum walk, so that the state function Ψ resides in $\ell^2(\mathbb{Z} \times \{R, L\})$. Let $\{|x\rangle|\sigma\rangle : x \in \mathbb{Z}, \sigma \in \{R, L\}\}$ be an orthonormal basis for $\ell^2(\mathbb{Z} \times \{R, L\})$. The degree of freedom $\{R, L\}$ is referred to as *chirality* or *spin*. Note that we represent the amplitude $\Psi(x)$ at each position $x \in \mathbb{Z}$ as a vector $\begin{bmatrix} \Psi_R(x) \\ \Psi_L(x) \end{bmatrix}$. This new underlying space allows us to formally define a quantum walk operator:

Definition 1.2 Let $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ be a unitary matrix. We define the one-dimensional two-state quantum walk operator $Q : \ell^2(\mathbb{Z} \times \{R, L\}) \rightarrow \ell^2(\mathbb{Z} \times \{R, L\})$ as $Q = T \circ (I \otimes U)$ where

$$(I \otimes U) : |n\rangle|R\rangle \mapsto a|n\rangle|R\rangle + c|n\rangle|L\rangle, \quad (I \otimes U) : |n\rangle|L\rangle \mapsto b|n\rangle|R\rangle + d|n\rangle|L\rangle \quad (1.2)$$

and

$$T : |n\rangle|R\rangle \mapsto |n+1\rangle|R\rangle, \quad T : |n\rangle|L\rangle \mapsto |n-1\rangle|L\rangle. \quad (1.3)$$

In particular, if $\Psi \in \ell^2(\mathbb{Z} \times \{R, L\})$ we can write:

$$(I \otimes U)\Psi(x) = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} \Psi_R(x) \\ \Psi_L(x) \end{bmatrix}, \quad T\Psi(x) = \begin{bmatrix} \Psi_R(x-1) \\ \Psi_L(x+1) \end{bmatrix}. \quad (1.4)$$

The quantum walk can be defined in a natural way on groups, as first suggested by Acevedo et. al. [3]:

Definition 1.3 Let (G, \cdot) be a group, let $\Sigma \subset G$ with $|\Sigma| = n$, and let $U \in U(n)$ where $U(n)$

is the set of $n \times n$ unitary matrices. The quantum walk operator $Q : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ corresponding to the triple (G, Σ, U) may be written as the composition $Q = T \circ (I \otimes U)$, where for $g \in G$ and $\sigma \in \Sigma$, $T : |g\rangle|\sigma\rangle \mapsto |g \cdot \sigma\rangle|\sigma\rangle$. We denote this correspondence as $Q \leftrightarrow (G, \Sigma, U)$.

In this form, the quantum walk operator in definition 2 can be written as $Q \leftrightarrow (\mathbb{Z}, \{-1, 1\}, U)$. The ordered pair (G, Σ) can be thought of as an undirected Cayley graph which admits loops [24]. We could define the quantum walk more generally as a triple (S, S', U) , where $S' \subset S$ and S is a set equipped with a binary operation (i.e. some function $\varphi : S \times S \rightarrow S$). Thus if $s \in S$ and $s' \in S'$, we define the translation operator in this case as $T : |s\rangle|s'\rangle \mapsto |\varphi(s, s')\rangle|s'\rangle$. However, we will choose to define the quantum walk directly on groups as above, as this standardizes the definition and automatically allows the operator Q to have an inverse.

In this thesis, we will primarily study quantum walks on $G = \mathbb{Z}$ or $G = \mathbb{Z}^2$, as has been considered in the literature ([9],[43],[65],[40]). Let $C_d \subset \mathbb{Z}^d$ be the standard set of unit vectors (cardinal directions in \mathbb{Z}^d), and let $\tilde{C}_d = C_d \cup \{0\}$. We will often take $\Sigma = C_d$ or $\Sigma = \tilde{C}_d$. The standard unitary matrices U studied in the quantum walk include the Hadamard matrix $H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ and the $n \times n$ Grover matrix $G_n = \frac{2}{n} \mathbf{1}_n - I_n$, where $\mathbf{1}_n$ is the $n \times n$ matrix of all ones. A quantum walk is governed by one of these two unitaries will be referred to as a *Hadamard walk* or a *Grover walk* respectively.

Quantum walks were considered in the literature as early as 1986, in an article by R.P. Feynman discussing potential quantum mechanical computers [29]. It was not until 1993 in a paper by Abrahamov that the discrete quantum walk was explicitly named and defined [5]. It should be noted that, due to its origins in computer science, there is great interest in defining the quantum walk on arbitrary graphs. While this is difficult in the discrete time case, continuous time quantum walks can be simply defined on graphs ([28], [31]). For a broader introduction to quantum walks, we direct the reader to two excellent articles by Kempe [40] and Venegas-Andraca [65]. For a more purely mathematical view, Konno [43]

is recommended.

As random walks are pervasive in classical computing algorithms ([52],[46],[59],[25],[26]), there has been extensive investigation into the use of quantum walks in quantum computing algorithms. Some algorithms in which the quantum walk plays a central role include the Grover search algorithm ([33],[58]) and Ambainis's algorithm for determining element distinctness [8]. It has in fact been proven by (Childs et. al. [22]) that the quantum walk is a universal computational primitive, i.e. any quantum computational algorithm can be formulated as a quantum walk. The quantum walk has also been physically realized in systems with a small number of qubits [66]. For more general information on quantum computation we direct the reader to [54].

This thesis is generally motivated by three main questions. First, what can we say about the asymptotic behavior of quantum walks on \mathbb{Z}^d ? Second, can one more generally describe absorption probabilities of quantum walks on \mathbb{Z} ? Last, how do quantum walks behave on finite domains, and in particular on finite domains with absorbing boundaries? The following three chapters will respectively treat these questions.

In Chapter 2 we discuss asymptotic behavior of quantum walks on \mathbb{Z}^d . In particular, we state the following main conjecture:

Conjecture 1.1 *Let $Q \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ be a quantum walk operator with $\Sigma = \{\sigma_1, \dots, \sigma_n\}$ with arbitrary initial condition, and let $\Psi_\sigma(x, t)$ be the amplitude of $Q^t \Psi$ at $|x\rangle|\sigma\rangle$. Then there exists a set $S \subset \mathbb{R}^d$ such that if $y \in S^\circ$ (the interior of S), then $\Psi_\sigma(yt, t) = \Omega(t^{-d/2})$, and if $y \notin \bar{S}$ (the closure of S), then $\Psi_\sigma(yt, t) = O(t^{-n})$ for every $n > 0$ (i.e. this quantity decays faster than any inverse power of t).*

Here, we say that $f(x) = \Omega(g(x))$ as $x \rightarrow \infty$ if there exists some $c > 0$ and a positive real x_0 such that for all $x > x_0$, we have $f(x) \geq cg(x)$. We refer to the set S as the *region of polynomial decay*. In Chapter 2, we refine and prove this conjecture for all walks in one dimension.

We can express the operator Q in Fourier space as a matrix multiplication operator

(whose terms involve the Fourier transform variable θ). For large integer t , the operator Q^t can then be studied by diagonalizing the multiplication matrix $M(\theta)$, with very strict care given to the analyticity properties (in θ) of the eigenvalues and eigenspaces of $M(\theta)$. We finally invert the Fourier transform applying the method of stationary phase to the resulting integrals. The selection of smooth or analytic eigenvalues of Q as functions of the Fourier parameter θ is the critical step here, and allows for the resolution of the conjecture in one dimension and pointing the way to its solution in higher dimensions as well.

In the remainder of Chapter 2 we provide detailed examples that demonstrate the conjecture and its proof in one dimension. We prove a precise asymptotic expansion of the (\mathbb{Z}, C_1, U) quantum walk distribution. If U is a general 2×2 unitary matrix written as $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$, we show that the region of polynomial decay is the interval $(-|a|, |a|)$. Two simultaneous papers by Nayak et. al. [53] and Ambainis et. al. [9] published in 2000-2001 give similar formulas for the special case of the (\mathbb{Z}, C_1, H) Hadamard walk. Konno ([41],[42],[43]) later provided a weak limit (in large time) of the probability distribution of the (\mathbb{Z}, C_1, U) quantum walk. However, these results did not include any oscillatory components of the asymptotic expansion of the state function, as is done here. For the $(\mathbb{Z}, \tilde{C}_1, G_3)$ Grover walk, we also compute the region of polynomial decay and we prove the phenomenon of *localization* for this walk. This occurs when the time averaged probability of the walker's returning to the origin does not vanish for large time and instead attains an asymptotic non-zero value.

We also study the corresponding regions of polynomial decay for two dimensional walks. The first paper to study quantum walks in higher dimensions was Mackay et. al. [49]. This was the first to observe localization in quantum walks governed by Grover matrices. Inui et. al. [36] characterized localization in the (\mathbb{Z}^2, C_2, G_4) Grover walk, and Watabe et. al. [68] performed a more precise calculation of the asymptotic behavior of such two-dimensional Grover walks. Baryshnikov et. al. [14] analyzed two dimensional quantum walks using differential geometric methods, while other authors have reviewed quantum

walks on non-Cartesian grids [1]. In Chapter 2 we study the global behavior of several widely studied walks, by identifying analytically their regions of polynomial decay. We study such behavior for the (\mathbb{Z}^2, C_2, G_4) Grover walk, the $(\mathbb{Z}^2, \tilde{C}_2, G_5)$ five-state Grover walk, the hexagonal Grover walk, and the $(\mathbb{Z}^2, C_2, H \otimes H)$ Hadamard walk.

As a final component of Chapter 2, we briefly discuss space-time inhomogeneous quantum walks whose transition operators are time and space dependent. We find (numerically for time-inhomogeneous quantum walks and analytically for space-inhomogeneous quantum walks) that when these dependences are periodic, the quantum walk exhibits its characteristic ballistic (linear spatial) spread asymptotically in time. However, if the inhomogeneities are aperiodic, the evolution of the quantum walk distribution alters drastically. In the time inhomogeneous case, it is possible for the distribution to evolve in a way that is parallel to the classical random walk, with a standard deviation growth of $O(\sqrt{t})$. For spatially inhomogeneous walks, an aperiodic position-dependent quantum walk operator can lead to so-called Anderson localization, which is often observed in sufficiently disordered quantum systems. Such results on inhomogeneous walks have previously been considered separately ([20],[57]).

In Chapter 3 we study the absorption problem for several classes of quantum walks. To discuss quantum walks with absorbing boundaries, we must first discuss quantum measurement. Consider the quantum walk operator $Q \leftrightarrow (G, \Sigma, U)$ and let $b \in G \times \Sigma$. We define the “yes” measurement operator $\Pi_{\text{yes}}^b : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ to be an orthogonal projection onto $|b\rangle$ while the “no” measurement operator $\Pi_{\text{no}}^b : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ projects onto the orthocomplement. The probabilistic interpretation of quantum mechanics states that if we measure a state Ψ at $|b\rangle$, then the state undergoes a ‘measurement collapse transition’ consisting of the projection $\frac{\Pi_{\text{yes}}^b \Psi}{\|\Pi_{\text{yes}}^b \Psi\|}$ with probability $\|\Pi_{\text{yes}}^b \Psi\|^2$, and the complementary projection $\frac{\Pi_{\text{no}}^b \Psi}{\|\Pi_{\text{no}}^b \Psi\|}$ with probability $\|\Pi_{\text{no}}^b \Psi\|^2$. If $B \subset G \times \Sigma$, we let Π_{no}^B be the composition of all *no* measurements at $b \in B$. We now define the absorbing quantum walk operator:

Definition 1.4 Let $Q \leftrightarrow (G, \Sigma, U)$ be a quantum walk operator and let $B \subset G \times \Sigma$. We say $\Pi_{no}^B Q$ is the absorbing quantum walk operator associated with the ordered quadruple (G, Σ, U, B) . We denote this correspondence by $\Pi_{no}^B Q \leftrightarrow (G, \Sigma, U, B)$.

Note that we do not re-normalize the absorbing quantum walk operator to maintain a conservation of probability in the total system i.e., norm 1 of the resulting vector. This is done to maintain linearity of the operator - such a normalization can then be done once the final state is reached. The absorption problem that is of interest here may be stated precisely as follows: let $\Pi_{no}^B Q \leftrightarrow (G, \Sigma, U, B)$ be an absorbing quantum walk operator and let $B_0 \subset B$. We wish to compute the probability P that the absorbing walk particle in initial state Ψ_0 is absorbed by B_0 before any other element in $B \sim B_0$. We can write this probability as:

$$P = \sum_{t=1}^{\infty} \left[\sum_{b \in B_0} |\langle b | Q (\Pi_{no}^B Q)^{t-1} | \Psi_0 \rangle|^2 \right]. \quad (1.5)$$

The above paper by Ambainis et. al. [9] was also the first to discuss absorption in quantum walks. Let p_{∞} be the probability associated with the $(\mathbb{Z}, C_1, H, \{0\})$ Hadamard walk (i.e. absorption of eventual absorption at $|0\rangle$ given an initial state of $|1\rangle|R\rangle$; here $B = B_0 = \{0\}$), and let p_n be the probability associated with the $(\mathbb{Z}, C_1, H, \{0, n\})$ Hadamard walk (i.e. the probability of eventual absorption at $|0\rangle$ given an initial state of $|1\rangle|R\rangle$ and another absorbing boundary at $|n\rangle$; here $B = \{0, n\}$ and $B_0 = \{0\}$). Ambainis et. al. proved the surprising fact that

$$\lim_{n \rightarrow \infty} p_n = \frac{1}{\sqrt{2}} > \frac{2}{\pi} = p_{\infty}. \quad (1.6)$$

That is, placing an additional absorbing boundary far away from the initial position in fact increases the probability of eventual left absorption. This indicates that absorbing boundaries in the quantum setting not only absorb but also reflect information.

Ambainis et. al. additionally conjectured a recurrence relation on the set of finite ab-

sorption probabilities, in the form

$$p_{n+1} = \frac{1 + 2p_n}{2 + 2p_n}. \quad (1.7)$$

It was not until 2009, in a work by Bach and Borisov [12] that this conjecture was proved using involved methods from complex analysis. These authors also considered recurrence relations for absorption probabilities for quantum walk states initialized at $|m\rangle|R\rangle$, and found a third order linear recurrence in terms of initial position m . A recent paper by Wang et. al. [67] used a similar complex analytic procedure to calculate absorption probabilities for the $(\mathbb{Z}, \tilde{C}_1, G_3, \{0, n\})$ absorbing Grover walk.

In Chapter 3 we extend the techniques originally developed by Bach and Borisov to study absorption probabilities for the $(\mathbb{Z}, C_1, U, \{0\})$ and $(\mathbb{Z}, C_1, U, \{0, n\})$ absorbing quantum walks with general unitary U and general initial condition. In particular, if $P_n^{(m)}(\alpha, \beta)$ is the probability that a particle initialized at $|m\rangle(\alpha|R\rangle + \beta|L\rangle)$ is eventually absorbed at $|0\rangle$ in the presence of an absorbing boundary at $|n\rangle$, we develop the following two relations:

Theorem 1.1 *For a finite one dimensional absorbing quantum walk with general unitary transition matrix $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ and initial condition $|m\rangle(\alpha|R\rangle + \beta|L\rangle)$, the absorption probabilities $P_n^{(m)}(\alpha, \beta)$ satisfy the recurrence*

$$P_{n+1}^{(m)}(1, 0) = \frac{|b|^2 + P_n^{(m)}(1, 0)}{1 + P_n^{(m)}(1, 0)} \quad (1.8)$$

in terms of the location of the right absorbing boundary n . Further,

$$P_n^{(m+3)}(\alpha, \beta) - \left(\frac{4}{|a|^2} - 1\right) P_n^{(m+2)}(\alpha, \beta) + \left(\frac{4}{|a|^2} - 1\right) P_n^{(m+1)}(\alpha, \beta) - P_n^{(m)}(\alpha, \beta) = 0. \quad (1.9)$$

Note that each of these recurrences determines the set of all absorption probabilities in one parameter (n or m) in terms of its first few values. We also prove similar results regarding

the absorption probabilities associated with the finite one dimensional absorbing Grover walk $(\mathbb{Z}, \tilde{C}_1, G_3, \{0, n\})$:

Theorem 1.2 *Let $P_n^{(m)}(\alpha, \beta, \gamma)$ be the probability that a particle initialized at $|m\rangle(\alpha|R\rangle + \beta|S\rangle) + \gamma|L\rangle$ is eventually absorbed at $|0\rangle$ in the presence of an absorbing boundary at $|n\rangle$. Then:*

$$P_{n+1}^{(m)}(1, 0, 0) = \frac{2 + 3P_n^{(m)}(1, 0, 0)}{3 + 4P_n^{(m)}(1, 0, 0)} \quad (1.10)$$

$$P_n^{(m+6)} - 134P_n^{(m+5)} + 3599P_n^{(m+4)} - 6932P_n^{(m+3)} + 3599P_n^{(m+2)} - 134P_n^{(m+1)} + P_n^{(m)} = 0 \quad (1.11)$$

Here, $P_n^{(m)} = P_n^{(m)}(\alpha, \beta, \gamma)$.

These explicit recurrences generalize those conjectured by Ambainis et. al. [9] for the Hadamard walk, and allow an explicit calculation of finite absorption probabilities. We also discuss possible methods for computing absorption probabilities for higher dimensional quantum walks.

In the final chapter (Chapter 4) we prove results regarding the long term behavior of quantum walks on finite domains, conditioned on non-absorption on the boundaries. This is an interesting problem both in the classical and quantum domain. Such behavior determined by eigenvalues and eigenvectors of the quantum walk operator. Let $Q_n \leftrightarrow (\mathbb{Z}, C_1, U, \{1, n\})$ be the absorbing quantum walk operator associated with a lattice of size n . If $p_n(\lambda)$ is the characteristic polynomial of Q_n , then we show that the sequence $\{p_n(\lambda)\}$ satisfies the second order recurrence:

$$p_{n+1}(\lambda) = (\lambda^2 + 1)p_n(\lambda) + |a|^2\lambda^2p_{n-1}(\lambda). \quad (1.12)$$

In general, it is impossible to compute the roots of $p_n(\lambda)$ using only elementary functions,

but the spectrum of Q_n is necessary to study the asymptotics of the confined (absorbing) walk.

Theorem 1.3 *Let $\Theta_n = \{\theta \in \mathbb{C} : \sin n\theta = \pm i \frac{|a|}{|b|} \sin \theta, |\operatorname{Re}(\theta)| \leq \pi\}$. The set Λ_n of eigenvalues of Q_n is:*

$$\Lambda_n = \{0\} \cup \{|a| \cos \theta \pm \sqrt{1 - |a|^2 \cos^2 \theta}, \theta \in \Theta_n\}. \quad (1.13)$$

We show these eigenvalues (with the exception of the double eigenvalue at $\lambda = 0$) uniformly approach the unit circle as the domain size n increases. These eigenvalues do not lie directly on the unit circle as the operator Q_n is no longer unitary. We also compute the eigenvectors of Q_n numerically, showing that the eigenvector corresponding to the k^{th} highest magnitude eigenvalue is $\frac{k}{2}$ periods of a sine wave (on the interval $[0, n]$ of integers) up to a phase, independent of the unitary matrix U . This shows the probability distribution of an absorbing quantum walk (conditioned on not being absorbed by the boundaries) approaches a squared sine wave at large time.

For the classical walk, we show that the analogous problem can be solved using Chebyshev polynomials [62]. There is a canonical correspondence between this discrete system with absorbing boundaries and the heat equation on the line with two heat sinks. Since the discrete quantum walk has no immediate PDE representation, it is not surprising that the computation of the eigenvalues and eigenvector components of the finite quantum walk is more involved than those of its classical counterpart. The classical random walk transition matrix has eigenvalues on the interval $(-1, 1)$, and its eigenvectors have entries that are discrete samplings of sine functions with integer periods. Comparing the structure of these eigenvalues to those of Q_n , we show that the absorbing quantum walk takes longer to reach a stability than the absorbing random walk.

Later in Chapter 4 we extend these results for two state absorbing quantum walks to the one dimensional finite Grover walk with absorbing boundaries. There we find eigenvalues that equal 1, yielding a precise description of above-mentioned localization. In an

exploratory search for the same phenomena in two dimensions, we study numerically the corresponding behavior of two dimensional quantum walks with corresponding absorbing boundaries (now in the form of boxes) under a variety of absorption schemes.

In the final portion of Chapter 4, we study what we denote as *modal phenomena*, in the conditional probability distributions of absorbing quantum walks. While the highest eigenvectors describe the long term behavior of conditional probability distributions for absorbing quantum walks, we show numerically that on smaller time scales the distributions evolve in very novel ways. At regular intervals, these distributions exhibit evenly spaced and sized peaks (modes). While the mechanism behind this behavior is the subject of future work, we numerically determine the behavior of the entropy of the conditional distribution over time.

The quantum walk is a relatively simple unitary discrete process with nontrivial behavior; however properties of this walk are often surprising and paradoxical in comparison to parallel ones for the classical random walk. In this work, we aim to prove precise results on the general two state one dimensional quantum walk and extrapolate these results to to more general classes of quantum walks.

Chapter 2

Asymptotic Behavior of Infinite Quantum Walks

The quantum walk differs fundamentally from classical random walks in a number of ways, for example the first grows linearly while the second spreads as the square root of time. Using stationary phase approximations, precise asymptotics have been derived for one-dimensional two-state quantum walks [41], one-dimensional three-state Grover walks [37], and two-dimensional four-state Grover walks [36]. In this paper we will extend these asymptotics to a conjecture for the d -dimensional case with arbitrary unitary transitions. We then prove this conjecture in one dimension. We also study numerically the regions of polynomial time-decay for several two-dimensional walks. We will also discuss long term behavior of inhomogeneous quantum walks (those with time and space dependent Hamiltonians) and show that periodic inhomogeneities lead to ballistic evolution (with time-linear dispersion) while aperiodic inhomogeneities result in distinctly non-quantum behavior.

2.1 Introduction

The quantum walk is a quantum mechanical analogue to the classical random walk. Its most basic formulation is the two-state walk in one dimension. Here, the state Ψ of the particle is an element of the space $\ell^2(\mathbb{Z} \times \{R, L\})$ where the two-state set $\{R, L\}$ refers to the *spin* or *chirality* of the particle. A single iteration is a two step process. First a unitary transformation (in this case a 2×2 matrix), or coin, is applied to the two spin components at each position. Second, amplitudes with a right spin component $|R\rangle$ are translated one

one unit in the positive x direction while amplitudes with a left spin component $|L\rangle$ are translated one step in the negative x direction.

Classical random walks have been used in classical computational algorithms [52][25] [26] and in particular for constructing search algorithms [59]. Often quantum walks can be used in quantum computational algorithms [58] [54] [29] to speed up the corresponding classical algorithms. The Grover search algorithm [33] can be formulated as a quantum walk and offers a quadratic speedup over the classical search algorithm. It has also been shown (Childs [22]) that the quantum walk is a universal computational primitive, so any quantum algorithm can be shown equivalent to a quantum walk, using a polynomial time transformation.

It is important to understand the quantum walk in a mathematical context parallel to its classical counterpart, independently of its utility in quantum computation. An initial effort in this direction was made by Ambainis et. al. [9] in a paper that provided a detailed asymptotic description of the Hadamard walk for large time. The large time behavior of the quantum walk contrasts with that of the classical walk [60] in both the shape of the probability density and rate of spread. Ambainis et. al. showed that the extent (standard deviation) of the Hadamard walk grows at $O(t)$ and in particular the distribution at time t is almost entirely contained in the interval $[-\frac{t}{\sqrt{2}}, \frac{t}{\sqrt{2}}]$. In this interval, the distribution contains highly oscillatory peaks at the edges and is approximately uniform near the origin. Compare these results to the classical walk, whose density approximates a normal at large time and has a standard deviation growing as $O(\sqrt{t})$.

These results were among the first in a line of papers describing asymptotic behavior of Hadamard and more general quantum walks. A few years later, Konno et. al. [41] extended these results to two state quantum walks with a general unitary coin. Inui et. al. [37] provided asymptotic results on the three-state one dimensional Grover walk with a focus on localization phenomena. Analysis of two-dimensional quantum walks started with a brief analysis by Mackay et. al. [49], and continued with a description of localization in the two-dimensional Grover walk by Inui [36], and a differential geometric interpretation

of two-dimensional quantum walks by Baryshnikov et. al. [14]. The asymptotic behavior of the one dimensional Hadamard walk described by Ambainis et. al. has served as a common baseline through these papers. The standard deviation of these walks grows as $O(t)$, and the probability distributions are almost entirely contained in a linearly expanding subset of the domain.

Some authors have generalized the quantum walk by considering temporal and spatial inhomogeneities in the transition operator Q . Brun et. al. [18] were the first to explore quantum walks governed by multiple coins. Ribeiro et. al. [57] found that applying a nonconstant periodic sequence of coins led to a quantum walk retaining ballistic spread, while applying an aperiodic sequence caused the probability distribution to exhibit the slower diffusive behavior of the classical walk. Cantero et. al. [19] studied the behavior of a quantum walk with isolated spatial defects, while Cedzich et. al. [20] showed that the so-called electric quantum walk eventually exhibits ballistic spread for walk parameters $\theta \in 2\pi\mathbb{Q}$ (yielding periodic spatial inhomogeneities) while the behavior sharply diverges for $\theta \notin 2\pi\mathbb{Q}$.

In this paper we provide a framework for the previously cited results and attempt to make more powerful claims about “quantum behavior” in quantum walks. In particular we present our results to support the following two conjectures:

Conjecture 2.1 *Let Q be an arbitrary quantum walk operator defined on \mathbb{Z}^d with arbitrary initial condition and let $\Psi_\sigma(x, t)$ be the amplitude at $|x\rangle|\sigma\rangle$ at time t . There exists a set $S \subset \mathbb{R}^d$ such that if $y \in S^\circ$ then $\Psi_\sigma(yt, t) = \Omega(t^{-d/2})$, and if $y \notin \bar{S}$, then $\Psi_\sigma(yt, t) = O(c^{-t})$ for some $c > 1$.*

Above, S° denotes the interior of S while \bar{S} denotes its closure. Also, \mathbb{Z}^d denotes the d -dimensional lattice based on the integers \mathbb{Z} , on which the state of the quantum walk is a function $\Psi(x, t) : \mathbb{Z}^d \times \mathbb{Z} \rightarrow \mathbb{C}^2$. We will prove a version of Conjecture 2.1 in one dimension.

We will briefly first define a more general quantum walk on groups that links together a variety of its versions. For space-time homogenous cases on \mathbb{Z} a quantum walk operator on

$\ell^2(\mathbb{Z} \times \{R, L\})$ is simply a linear combination of translation operations. We can thus Fourier transform to find that the transformed operator is a multiplication by a variable matrix in Fourier space. Thus iterations of the quantum walk operator correspond to raising this Fourier multiplier matrix to a power. We use a spectral matrix decomposition together with an inverse Fourier transform, using the asymptotics of the method of stationary phase [17] [61]. In one dimension we find precise asymptotics and confirm that the probability distribution of the quantum walk nearly vanishes outside a linearly expanding region (the set S in Conjecture 2.1) which we term the *region of polynomial decay*. While the one dimensional results cited previously are concerned with analytic results, their stationary phase approximations become unwieldy in higher dimensions. Thus, for some additional two dimensional walks we will only attempt to analyze regions of polynomial decay. We conclude by providing some insights into parallels and differences with spatially and temporally inhomogeneous quantum walks and analyzing why aperiodic inhomogeneities cause their behavior to differ so sharply from their homogeneous counterparts.

The rest of the paper is organized as follows. The definition of the walk and a discussion of Fourier transforms and stationary phase are in Section 2.2. Section 2.3 discusses precise asymptotic expansions of one dimensional walks, and in section 2.4 we identify regions of nondecay for several higher dimensional walks. We review inhomogeneous quantum walks in Section 2.5.

2.2 Definitions and Methods

We begin by defining the quantum walk on a group, as first introduced by Acevedo et. al. [3]:

Definition 2.1 *Let (G, \cdot) be a group, let $\Sigma \subset G$ with $|\Sigma| = n$, and let $U \in U(n)$ where $U(n)$ is the set of $n \times n$ unitary matrices. The quantum walk operator $Q : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ corresponding to the triple (G, Σ, U) may be written as the composition $Q = T \circ (I \otimes U)$ where for $g \in G$ and $\sigma \in \Sigma$, $T : |g\rangle|\sigma\rangle \mapsto |g \cdot \sigma\rangle|\sigma\rangle$. We denote this correspondence as*

$$Q \leftrightarrow (G, \Sigma, U).$$

The ordered pair (G, Σ) can be thought of as an undirected Cayley graph which admits loops [24]. In this paper, we will primarily consider $G = \mathbb{Z}$ or \mathbb{Z}^2 . Let $C_d \subset \mathbb{Z}^d$ be the set of unit directional vectors in \mathbb{Z}^d and let $\tilde{C}_d = C_d \cup \{0\}$. The unitary transition matrices we use include arbitrary 2×2 unitary matrices $\begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ ($|a|^2 + |b|^2 = 1$) and the $n \times n$ Grover matrix $G_n = \frac{2}{n}\mathbf{1}_n - I_n$ with $\mathbf{1}_n$ the $n \times n$ matrix filled with ones and I_n the $n \times n$ identity matrix.

One way to view this quantum walk operator is as a linear combination of translations. Let $\psi \in \ell^2(G)$ and let $T_\sigma : \ell^2(G) \rightarrow \ell^2(G)$ with $\sigma \in \Sigma$ be a translation operator which acts by $T_\sigma(\psi(g)) = \psi(g \cdot \sigma^{-1})$. Then we can visualize Q acting on the vector $[\psi_{\sigma_1}, \dots, \psi_{\sigma_n}]'$ as follows:

$$Q = \begin{bmatrix} T_{\sigma_1} & & \\ & \ddots & \\ & & T_{\sigma_n} \end{bmatrix} U. \quad (2.1)$$

When $G = \mathbb{Z}^d$, we can gain a better understanding of Q through the application of a Fourier transform. We define the discrete Fourier transform as follows:

Definition 2.2 *The discrete Fourier transform of $f : \mathbb{Z}^d \rightarrow \mathbb{C}$ is:*

$$\mathcal{F}[f](\theta) = \sum_{x \in \mathbb{Z}^d} f(x) e^{ix \cdot \theta}.$$

As usual this is an isometry from $\ell^2(\mathbb{Z}^d)$ to $L^2([-\pi, \pi]^d)$. The inverse transform is then:

$$\mathcal{F}^{-1}[\hat{f}](x) = \frac{1}{(2\pi)^d} \int_{\|\theta\|_\infty < \pi} \hat{f}(\theta) e^{-ix \cdot \theta} d\theta,$$

where $\theta = (\theta_1, \dots, \theta_d)$ and $\|\theta\|_\infty = \sup |\theta_i|$.

We will now conjugate the quantum walk with the Fourier transform to investigate its

dynamics in Fourier space. Let $f : \mathbb{Z}^d \rightarrow \mathbb{C}$ and $\sigma \in \mathbb{Z}^d$. Then:

$$\begin{aligned} \mathcal{F}[T_\sigma f](\theta) &= \sum_{x \in \mathbb{Z}^d} f(x - \sigma) e^{ix \cdot \theta} \\ &= e^{i\sigma \cdot \theta} \sum_{x \in \mathbb{Z}^d} f(x - \sigma) e^{i(x - \sigma) \cdot \theta} \\ &= e^{i\sigma \cdot \theta} \mathcal{F}[f](\theta). \end{aligned}$$

Under Fourier conjugation the translation operator acts as a multiplication operator, and:

$$\mathcal{F}[Q\Psi] = \begin{bmatrix} e^{i\sigma_1 \cdot \theta} & & \\ & \ddots & \\ & & e^{i\sigma_n \cdot \theta} \end{bmatrix} U\mathcal{F}[\Psi] \equiv M(\theta)\mathcal{F}[\Psi]. \quad (2.2)$$

We refer to $M(\theta)$ above as the *multiplier matrix*.

Clearly the quantum walk now involves raising (Fourier position-dependent) matrices to high powers in Fourier space. If $\{\lambda_j(\theta)\}_{j=1}^n$ is the set of eigenvalues of $M(\theta)$ we can write for a quantum walk with initial condition Ψ_0 :

$$M(\theta)^t \mathcal{F}[\Psi_0] = \sum_{j=1}^n \lambda_j(\theta)^t E_j(\theta).$$

Here, the $E_j(\theta)$ are scaled eigenvectors that depend on $\mathcal{F}[\Psi_0]$ and are a byproduct of the eigenvalue decomposition. Furthermore, since $M(\theta)$ is unitary, we can write $\lambda_j(\theta) = e^{i\Xi_j(\theta)}$ where $\Xi_j : [-\pi, \pi]^d \rightarrow \mathbb{R}$. Inverse transforming:

$$Q^t \Psi = \frac{1}{(2\pi)^d} \sum_{j=1}^n \int_{\|\theta\|_\infty \leq \pi} E_j(\theta) e^{i(t\Xi_j(\theta) - x \cdot \theta)} d\theta.$$

By letting $x = yt$ where $y \in \mathbb{R}^d$, we have:

$$Q^t \Psi = \frac{1}{(2\pi)^d} \sum_{j=1}^n \int_{\|\theta\|_\infty \leq \pi} E_j(\theta) e^{it(\Xi_j(\theta) - y \cdot \theta)} d\theta. \quad (2.3)$$

Method of Stationary Phase

Having taken a large power of this matrix for study of asymptotics, we must invert the Fourier transform. We will do this analytically, using the method of stationary phase [17]. We illustrate this in detail on a domain of one dimension. When we take the d -dimensional inverse Fourier transform, we will consider integrals:

$$I(t) = \int_{\mathbb{R}^d} g(x)e^{itf(x)} dx, \quad (2.4)$$

for large values of t , with $g(x)$ and $f(x)$ smooth or analytic. Intuitively, $e^{itf(x)}$ oscillates rapidly when t is large, leading to extensive cancellations in the integral. This however does not hold in the neighborhood of a point $x \in \mathbb{R}^d$ such that $\nabla f(x) = 0$. We say that x satisfying this condition is a *point of stationary phase* or a *critical point*. We refer to the following three results in Stein [61]:

Proposition 2.1 *Suppose f and g are smooth real-valued functions, g has compact support, and f has no critical points in the support of g . Then $I(t) = O(t^{-n})$ for every $n \geq 0$.*

This follows directly from [61] (Proposition 2.1 in Section 8.2). This tells us that for oscillatory integrals involving smooth functions that contain no points of stationary phase, the integral has superpolynomial decay. The next proposition, also from [61], is a weakened version of the original that makes subsequent arguments more clear.

Proposition 2.2 *Suppose f and g are smooth, g has compact support, and for some multi-index α we have $|\partial_x^\alpha f| > 0$ throughout the support of g . Then $I(t) = O(t^{-1/|\alpha|})$.*

This follows directly from Proposition 5 in Section 8.2 in [61]. Above, for $f : \mathbb{R}^d \rightarrow \mathbb{R}$ and $\alpha = (\alpha_1, \dots, \alpha_d)$ a multi-index with nonnegative integer α_i , we have defined $\partial_x^\alpha f = \frac{\partial^{|\alpha|} f}{\partial x_1^{\alpha_1} \dots \partial x_d^{\alpha_d}}$, with $|\alpha| = \sum_i \alpha_i$. We note that this proposition gives only basic information about decay rates, and as suggested by Proposition 2.1, these rates may be much greater (if

there are no critical points). The decay rate in Proposition 2.2 can only be considered an upper bound. However, this statement will still be useful for us. We say that a critical point $x \in \mathbb{R}^d$ is *nondegenerate* if the matrix $\left[\frac{\partial^2 f}{\partial x_i \partial x_j} \right] (x)$ is invertible. The following Proposition [61] treats such cases:

Proposition 2.3 *Suppose f has a nondegenerate critical point at x_0 and g is supported in a sufficiently small neighborhood of x_0 . Then $I(t) = \Theta(t^{-d/2})$.*

We say that $g(x) = \Theta(f(x))$ if there exists $c_1, c_2, X > 0$ such that $c_1 f(x) \leq g(x) \leq c_2 f(x)$ for all $x > X$. For one dimensional integrals, we can explicitly write out corresponding asymptotic expressions. Let $f : \mathbb{R} \rightarrow \mathbb{R}$ and let $X = \{x \in \mathbb{R} : f'(x) = 0, f''(x) \neq 0\}$ be the set of all nondegenerate critical points. Suppose this set is finite and listed as $X = \{x_1, \dots, x_k\}$. Then we may write $I(t) = \sum_{j=1}^k I_j(t) + R(t)$ where $R(t) = O(t^{-1})$ ($t \rightarrow \infty$) and each summand $I_j(t)$ can be written as:

$$I_j(t) = g(x_j) e^{itf(x_j)} \sqrt{\frac{\pi}{t|f''(x_j)|}} (1 \pm i) \quad (2.5)$$

Here, the \pm sign is determined by the sign of $f''(x_j)$. This result is given in equation (12) of Section 8.1 in [61] and may be obtained directly from properties of Fresnel integrals [2].

To use the above stationary phase approximations, we must prove that the functions $\Xi_j(\theta)$ from equation (2.3) can be chosen to be smooth. To do this we require a result from Rainer [56].

Proposition 2.4 *Let $A(t) = (A_{ij}(t))$ be a smooth curve of complex $n \times n$ normal matrices depending on a real parameter $t \in \mathbb{R}$. Suppose that no two of the continuous eigenvalues meet to infinite order at any t if they are not equal for all t . Then all of the eigenvalues and eigenvectors can be chosen smoothly in t on the whole parameter domain.*

With these propositions, we are ready to prove the main theorem of this Chapter.

Theorem 2.1 *Let $Q \leftrightarrow (\mathbb{Z}, \Sigma, U)$ be a one dimensional quantum walk operator with $\Sigma =$*

$\{\sigma_1, \dots, \sigma_n\}$, having an arbitrary initial condition $|0\rangle (\alpha_1|\sigma_1\rangle + \dots + \alpha_n|\sigma_n\rangle)$, and let $\Psi(x, t)$ be the vector of amplitudes at $|x\rangle|\sigma\rangle$ for all $\sigma \in \Sigma$ at time t . There exists a set $S \subset \mathbb{R}$ such that if $y \notin S$ then $\Psi(yt, t) = O(t^{-N})$ for all $N > 0$. Furthermore, there exists a subset $A \subset S$ such that, if $y \in A$, then $\Psi(yt, t) = \Omega(t^{-1/2})$ for almost every choice of initial condition vector $\alpha = (\alpha_1, \dots, \alpha_n)$.

Proof: Recall equation (2.3):

$$\Psi(yt, t) = \frac{1}{2\pi} \sum_{j=1}^n \int_{-\pi}^{\pi} E_j(\theta) e^{it(\Xi_j(\theta) - y\theta)} d\theta.$$

Here, $\lambda_j(\theta) = e^{i\Xi_j(\theta)}$ is an eigenvalue of the unitary multiplier matrix

$$M(\theta) = \begin{bmatrix} e^{i\sigma_1 \cdot \theta} & & \\ & \ddots & \\ & & e^{i\sigma_n \cdot \theta} \end{bmatrix} U$$

which is smoothly parameterized by θ . Proposition 2.4 implies that we can choose $\lambda_j(\theta)$ to be smooth. Since $|\lambda_j(\theta)| = 1$ for all θ , we can choose a branch of the logarithm such that $\Xi_j(\theta)$ is also smooth. Moreover, the eigenvectors $E_j(\theta)$ of $M(\theta)$ can also be chosen to be smooth by Proposition 2.4. We thus conclude that the integral in (2.3) satisfies the conditions necessary to use stationary phase approximations.

Let $S = \cup_{j=1}^n \Xi'_j([- \pi, \pi])$ form the union of ranges $\Xi'_j(\theta) = \frac{d}{d\theta} \Xi(\theta)$. If $y \in S$, then for some j the exponent $f_j(\theta) = \Xi_j(\theta) - y\theta$ in equation (2.3) has a critical point. If $y \notin S$ however, $f_j(\theta)$ contains no critical points for any j . Thus, by Proposition 2.1, for $y \notin S$ the amplitudes $\Psi(yt, t)$ decay superpolynomially as $t \rightarrow \infty$. If we let $A_j = \{\theta \in (-\pi, \pi) : \Xi''_j(\theta) \neq 0\}$, then the choice $A = \cap_{j=1}^n \Xi'_j(A_j)$ allows us to satisfy the conditions of the theorem as per Proposition 2.3. One must consider the possibility that at all points y in the infinite set A above, there is a cancellation of the terms of the form (2.5) arising from the stationary phase approximations. However, because each of these terms is in fact

analytic in y (see proof of Theorem 2.3 below), this cannot occur at all such points y , leaving some y for which $|\Psi(ty, t)| = \Omega(t^{-1/2})$, with no cancellation of the leading terms (2.5). \square

We make note of the following definition in connection with the proof of this theorem:

Definition 2.3 *Let $Q \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ be a d -dimensional quantum walk operator with Fourier multiplier matrix $M(\theta_1, \dots, \theta_d)$, and let $\lambda_j(\theta_1, \dots, \theta_d) = e^{i\Xi_j(\theta_1, \dots, \theta_d)}$ be a smoothly varying eigenvector of $M(\theta_1, \dots, \theta_d)$. We define the set $S_j = (\nabla\Xi_j)([-\pi, \pi]^d)$ to be the region of polynomial decay with respect to the eigenvalue $\lambda_j(\theta_1, \dots, \theta_d)$. We define the union $S = \cup_{j=1}^n S_j$ to be the total region of polynomial decay.*

Since the smooth or analytic dependence of eigenvalues and eigenvectors on single parameters θ in Proposition 2.4 cannot easily be extended to hold for smooth maps on more than one dimension (see [Kato Section II.5.7 [39]]), the proof of Theorem 2.1 cannot directly be extended to similarly describe quantum walks in higher dimensions. However, in some higher dimensional cases it is possible to determine explicitly that eigenvalues depend analytically on θ , as will be done in examples below. In these cases identical arguments to those in one dimension (see Theorems 2.1, 2.3) will show that the region of polynomial decay (except possibly for a set of $y \in \mathbb{R}^2$ of measure 0) is a domain of polynomial decay of expected order, i.e. $\Omega(t^{-d/2})$ with d dimension. For the (\mathbb{Z}, C_1, U) quantum walk, we will use equation (2.5) to compute precise asymptotics. For the other homogeneous walks presented in the paper we will compute the regions of polynomial decay as defined above. For the two dimensional walks, for example. the function $\nabla\Xi_j$ will give us a parametric representation of this region. We can do this because the eigenvalues and eigenvectors can be chosen smoothly.

Finally we note that this theorem grants us slow decay rates on some subset $A \subset S$. An extension is considered in Theorem 2.3, which shows that for y in the above-defined region of polynomial decay the decay is precisely of order $t^{-1/2}$ for almost all initial conditions and all but at most a finite number of $y \in S$.

2.3 One Dimensional Walks

We first consider some preliminaries. For the one dimensional walks we will consider, a non-constant eigenvalue $\lambda(\theta)$ of the Fourier multiplier matrix $M(\theta)$ will satisfy a general quadratic equation of the form

$$\lambda(\theta)^2 - 2a(\theta)\lambda(\theta) + 1 = 0. \quad (2.6)$$

for a smooth function $a(\theta)$. Since $M(\theta)$ is unitary and depends analytically on θ , we can write $\lambda(\theta) = e^{i\Xi(\theta)}$, where $\Xi(\theta)$ is a smooth function of θ . Using implicit differentiation we obtain

$$\Xi'(\theta) = \frac{\lambda'(\theta)}{i\lambda(\theta)} = \frac{a'(\theta)}{i(\lambda(\theta) - a(\theta))}. \quad (2.7)$$

This will be a convenient method for representing regions of polynomial decay.

We will also need a convenient representation for our matrix powers:

Lemma 2.1 *Let $M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ be a 2×2 matrix, $\lambda_{\pm} = \frac{1}{2} \left[a + d \pm \sqrt{(a+d)^2 - 4(ad-bc)} \right]$, and $F_n = \lambda_+^n - \lambda_-^n$. Then we can write:*

$$M^n = \frac{1}{F_1} \begin{bmatrix} F_{n+1} - dF_n & bF_n \\ cF_n & F_{n+1} - aF_n \end{bmatrix}.$$

The (\mathbb{Z}, C_1, U) General Unitary One Dimensional Quantum Walk

We now generalize the large time asymptotic analysis of Ambainis et. al. [9] to study transition operators $Q \leftrightarrow (\mathbb{Z}, C_1, U)$ involving general unitary matrices U . We will parameterize a general 2×2 unitary matrix as

$$U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix} \quad (2.8)$$

with $|a|^2 + |b|^2 = 1$. Previous analyses of the asymptotic behavior of this more general two state walk ([41],[42],[43]) have not included the detailed asymptotics of the oscillatory components studied here.

The asymptotic analysis is somewhat nuanced, and we divide it into several steps. We are interested in the large time walk amplitude $\Psi(yt, t) = Q^t \psi$, in the region of polynomial (slow) decay for an initial condition $\Psi_0 = |0\rangle(\alpha|R\rangle + \beta|L\rangle)$, and $y \in \mathbb{R}$.

We first derive a closed form expression for the amplitudes, prior to developing a stationary phase approximation:

Lemma 2.2 *The quantities*

$$\lambda_{\pm}(\theta) \equiv e^{i\Xi_{\pm}(\theta)} = \text{Re}(ae^{i\theta}) \pm i\sqrt{1 - (\text{Re}(ae^{i\theta}))^2} \quad (2.9)$$

are eigenvalues of the multiplier matrix $M(\theta)$. Let:

$$E_{\pm}(\theta) = \pm \frac{1}{2\sqrt{1 - (\text{Re}(ae^{i\theta}))^2}} \begin{bmatrix} -\alpha(\lambda_{\mp}(\theta) - ae^{i\theta}) + \beta be^{i\theta} \\ -\alpha \bar{b}e^{-i\theta} + \beta(\lambda_{\pm}(\theta) - ae^{i\theta}) \end{bmatrix}. \quad (2.10)$$

Then:

$$\Psi(yt, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} E_{+}(\theta) e^{it(\Xi_{+}(\theta) - y\theta)} d\theta + \frac{1}{2\pi} \int_{-\pi}^{\pi} E_{-}(\theta) e^{it(\Xi_{-}(\theta) - y\theta)} d\theta. \quad (2.11)$$

Proof: From equation (2.2), we find that Q has the following Fourier representation:

$$\mathcal{F}[Q\psi](\theta) = \begin{bmatrix} ae^{i\theta} & be^{i\theta} \\ -\bar{b}e^{-i\theta} & \bar{a}e^{-i\theta} \end{bmatrix} \mathcal{F}[\psi](\theta) \quad (2.12)$$

where $M(\theta) = \begin{bmatrix} ae^{i\theta} & be^{i\theta} \\ -\bar{b}e^{-i\theta} & \bar{a}e^{-i\theta} \end{bmatrix}$. The eigenvalues $\lambda(\theta)$ of $M(\theta)$ satisfy:

$$\lambda(\theta)^2 - 2(\operatorname{Re}(ae^{i\theta}))\lambda(\theta) + 1 = 0, \quad (2.13)$$

of the same form as equation (2.6) above with two solutions $\lambda_{\pm}(\theta)$. Since $|\lambda_{\pm}(\theta)| = 1$ we write $\lambda_{\pm}(\theta) = e^{i\Xi_{\pm}(\theta)}$ with $\Xi_{\pm}(\theta)$ real.

We use Lemma 2.1 to write powers of $M(\theta)$:

$$\begin{bmatrix} ae^{i\theta} & be^{i\theta} \\ -\bar{b}e^{-i\theta} & \bar{a}e^{-i\theta} \end{bmatrix}^t = \frac{1}{F_1(\theta)} \begin{bmatrix} ae^{i\theta}F_t(\theta) - F_{t-1}(\theta) & be^{i\theta}F_t(\theta) \\ -\bar{b}e^{-i\theta}F_t(\theta) & F_{t+1}(\theta) - ae^{i\theta}F_t(\theta) \end{bmatrix},$$

with $F_t(\theta) = \lambda_+(\theta)^t - \lambda_-(\theta)^t$ as in Lemma 2.1. Suppose we have initial condition $\Psi_0 \equiv \Psi(0, 0) = [\alpha, \beta]'$ where $|\alpha|^2 + |\beta|^2 = 1$. Since $\mathcal{F}[\Psi_0] = [\alpha, \beta]'$, we can write $\mathcal{F}[Q^t\Psi_0]$ by multiplying $\mathcal{F}[\Psi_0]$ by the above matrix:

$$\mathcal{F}[Q^t\psi] = \frac{1}{F_1(\theta)} \begin{bmatrix} -\alpha(\lambda_-(\theta) - ae^{i\theta}) + \beta be^{i\theta} \\ -\alpha\bar{b}e^{-i\theta} + \beta(\lambda_+(\theta) - ae^{i\theta}) \end{bmatrix} \lambda_+(\theta)^n + \frac{1}{F_1(\theta)} \begin{bmatrix} \alpha(\lambda_+(\theta) - ae^{i\theta}) - \beta be^{i\theta} \\ \alpha\bar{b}e^{-i\theta} - \beta(\lambda_-(\theta) - ae^{i\theta}) \end{bmatrix} \lambda_-(\theta)^n. \quad (2.14)$$

using $\lambda_+(\theta)\lambda_-(\theta) = 1$. Note that these displayed vectors (including the $\frac{1}{F_1(\theta)}$ terms in front) equal $E_{\pm}(\theta)$. Inverse Fourier transforming and letting $x = yt$ gives the desired result.

□

To compute $\Psi(yt, t)$ asymptotically, we must now compute points of stationary phase for each integral in (2.8), which themselves depend on y . We have:

Lemma 2.3 *Let $S_{\pm}(y) = \{\theta \in [-\pi, \pi] : \Xi'_{\pm}(\theta) = y\}$ denote the points of stationary phase for the integral (2.8) as a function of the position variable $y \in \mathbb{R}$. Then if $|y| > |a|$, there are no points of stationary phase ($S_{\pm} = \emptyset$) and if $|y| < |a|$, S_+ and S_- each contain two points, so that $S_+ = \{\theta_{+1}, \theta_{+2}\}$ and $S_- = \{\theta_{-1}, \theta_{-2}\}$, so that $\Xi'_{\pm}(\theta_{\pm 1}) = \Xi'_{\pm}(\theta_{\pm 2}) = y$.*

The points $\theta_{\pm 1}$ and $\theta_{\pm 2}$ are given by:

$$\begin{aligned}
ae^{i\theta_{+1}} &= \sqrt{\frac{|a|^2 - y^2}{1 - y^2}} + i \frac{|b|y}{\sqrt{1 - y^2}}, & ae^{i\theta_{+2}} &= -\sqrt{\frac{|a|^2 - y^2}{1 - y^2}} + i \frac{|b|y}{\sqrt{1 - y^2}} \\
ae^{i\theta_{-1}} &= \sqrt{\frac{|a|^2 - y^2}{1 - y^2}} - i \frac{|b|y}{\sqrt{1 - y^2}}, & ae^{i\theta_{-2}} &= -\sqrt{\frac{|a|^2 - y^2}{1 - y^2}} - i \frac{|b|y}{\sqrt{1 - y^2}}.
\end{aligned} \tag{2.15}$$

Proof: Recall from equation (2.9) that the eigenvalues $\lambda_{\pm}(\theta) = e^{i\Xi_{\pm}(\theta)}$ of the Fourier multiplier matrix $M(\theta)$ satisfy $\lambda_{\pm}(\theta) = \text{Re}(ae^{i\theta}) \pm i\sqrt{1 - (\text{Re}(ae^{i\theta}))^2}$. Using equation (2.7) with $a(\theta) = \text{Re}(ae^{i\theta})$ and the aforementioned eigenvalues, we have:

$$\Xi'_{\pm}(\theta) = \pm \frac{\text{Im}(ae^{i\theta})}{\sqrt{1 - (\text{Re}(ae^{i\theta}))^2}}. \tag{2.16}$$

Note that $(\text{Re}(ae^{i\theta}))^2 + (\text{Im}(ae^{i\theta}))^2 = |a|^2$. By letting $\Xi'_{\pm}(\theta) = y$ and squaring both sides, we can write $(\text{Re}(ae^{i\theta}))^2$ in terms of y^2 :

$$(\text{Re}(ae^{i\theta}))^2 = \frac{|a|^2 - y^2}{1 - y^2}.$$

Proceeding to solve for θ in terms of y , the above equation has no solutions for $\theta \in [-\pi, \pi]$ if $|y| > |a|$, and two solutions for $|y| \leq |a|$. Let $ae^{i\theta_{\pm 1}}$ have nonnegative real part and $ae^{i\theta_{\pm 2}}$ have nonpositive real part. Plugging this into equation (2.16) gives us the full result. \square

Notice that this result tells us that for $|y| > |a|$ there are no points of stationary phase in the integrals of equations (2.8). Thus by Proposition 2.1 for such y there will be superpolynomial decay in $\Psi(yt, t)$. Correspondingly, we will expect polynomial decay for $|y| < |a|$, since for such values these integrals will have points of stationary phase whose first order asymptotic behaviors clearly do not cancel each other. Thus the region of polynomial decay associated with the eigenvalues $\lambda_{\pm}(\theta)$ of $M(\theta)$ is $y \in (-|a|, |a|)$. Equipped with implicit representations of the points of stationary phase, we must plug these into equation (2.5) to complete the approximation. We present a few of these substitutions as lemmas

here and omit proofs:

Lemma 2.4 *We have the following expressions for the eigenvalues $\lambda_{\pm}(\theta)$ of the matrix $M(\theta)$, evaluated at the points of stationary phase $\theta_{\pm 1}$ and $\theta_{\pm 2}$ for $|y| < |a|$:*

$$\begin{aligned}\lambda_+(\theta_{\pm 1}) &= \sqrt{\frac{|a|^2 - y^2}{1 - y^2}} + i \frac{|b|}{\sqrt{1 - y^2}}, & \lambda_+(\theta_{\pm 2}) &= -\sqrt{\frac{|a|^2 - y^2}{1 - y^2}} + i \frac{|b|}{\sqrt{1 - y^2}} \\ \lambda_-(\theta_{\pm 1}) &= \sqrt{\frac{|a|^2 - y^2}{1 - y^2}} - i \frac{|b|}{\sqrt{1 - y^2}}, & \lambda_-(\theta_{\pm 2}) &= -\sqrt{\frac{|a|^2 - y^2}{1 - y^2}} - i \frac{|b|}{\sqrt{1 - y^2}}.\end{aligned}\quad (2.17)$$

Lemma 2.5 *Recalling that the eigenvalues of $M(\theta)$ are $\lambda_{\pm}(\theta) = e^{i\Xi_{\pm}(\theta)}$ We have for $|y| < |a|$:*

$$\begin{aligned}\Xi_+''(\theta_{+1}) &= \frac{(1 - y^2)\sqrt{|a|^2 - y^2}}{|b|}, & \Xi_+''(\theta_{+2}) &= -\frac{(1 - y^2)\sqrt{|a|^2 - y^2}}{|b|} \\ \Xi_-''(\theta_{-1}) &= -\frac{(1 - y^2)\sqrt{|a|^2 - y^2}}{|b|}, & \Xi_-''(\theta_{-2}) &= \frac{(1 - y^2)\sqrt{|a|^2 - y^2}}{|b|}.\end{aligned}\quad (2.18)$$

Lemma 2.6 *We have the following expressions for $E_{\pm}(\theta)$ of equation (2.8) evaluated at the four critical points $\{\theta_{\pm 1}, \theta_{\pm 2}\}$:*

$$\begin{aligned}E_+(\theta_{+1}) &= \frac{1}{2} \left[\alpha(1 + y) + \frac{\beta b}{a} y - i \frac{\beta b}{a|b|} \sqrt{|a|^2 - y^2} \right. \\ &\quad \left. \frac{\alpha \bar{b}}{a} y + \beta(1 - y) + i \frac{\alpha \bar{b}}{a|b|} \sqrt{|a|^2 - y^2} \right] \\ E_+(\theta_{+2}) &= \frac{1}{2} \left[\alpha(1 + y) + \frac{\beta b}{a} y + i \frac{\beta b}{a|b|} \sqrt{|a|^2 - y^2} \right. \\ &\quad \left. \frac{\alpha \bar{b}}{a} y + \beta(1 - y) - i \frac{\alpha \bar{b}}{a|b|} \sqrt{|a|^2 - y^2} \right] \\ E_-(\theta_{-1}) &= \frac{1}{2} \left[\alpha(1 + y) + \frac{\beta b}{a} y + i \frac{\beta b}{a|b|} \sqrt{|a|^2 - y^2} \right. \\ &\quad \left. \frac{\alpha \bar{b}}{a} y + \beta(1 - y) - i \frac{\alpha \bar{b}}{a|b|} \sqrt{|a|^2 - y^2} \right]\end{aligned}\quad (2.19)$$

$$E_+(\theta_{+2}) = \frac{1}{2} \left[\alpha(1+y) + \frac{\beta b}{\alpha} y - i \frac{\beta b}{a|b|} \sqrt{|a|^2 - y^2} \right] \\ \left[\frac{\alpha \bar{b}}{a} y + \beta(1-y) + i \frac{\alpha \bar{b}}{a|b|} \sqrt{|a|^2 - y^2} \right].$$

We now combine these to explicitly describe the first order behavior of the amplitude $\Psi(yt, t)$ of the quantum walk in the limit $t \rightarrow \infty$. Recall that our initial condition is assumed to be $\Psi_0 = |0\rangle (\alpha|R\rangle + \beta|L\rangle)$:

Theorem 2.2 *Recall the relation $y = \Xi'_\pm(\theta)$, and the above two solutions $\theta = \theta_{\pm 1}(y)$ and $\theta = \theta_{\pm 2}(y)$. Let $f(y) = e^{i\theta_{+1}(y)}$, $g(y) = \lambda_+(\theta_{+1}(y))$ and let*

$E = \frac{1}{2} \left[\alpha(1+y) + \frac{\beta b}{a} y - i \frac{\beta b}{a|b|} \sqrt{|a|^2 - y^2} \right] \left[\frac{\alpha \bar{b}}{a} y + \beta(1-y) + i \frac{\alpha \bar{b}}{a|b|} \sqrt{|a|^2 - y^2} \right]$. For large t and for $|y| < |a|$, the quantum walk amplitude satisfies:

$$\Psi(yt, t) = 2(1 + (-1)^{t(1+y)}) \sqrt{\frac{\pi|b|}{t(1-y^2)\sqrt{|a|^2 - y^2}}} a^{ty} \operatorname{Re} \left[E e^{i\pi/4} \frac{g(y)^t}{f(y)^{yt}} \right] + R(t) \quad (2.20)$$

where for each y , $R(t) = O(t^{-1})$ as $t \rightarrow \infty$.

Proof: Let $E = E_+(\theta_{+1})$, $x = ae^{i\theta_{+1}}$, $\lambda = e^{i\Xi_+(\theta_{+1})}$, $z = 1 + i$, and $\Xi'' = |\Xi''_+(\theta_{+1})|$. This result is obtained through the following process of evaluating the oscillatory integrals (2.11) by applying (2.5) and combining the four points of stationary phase $\theta_{\pm 1}$ and $\theta_{\pm 2}$ in the two integrals of (2.11) (see Lemmas 2.4-2.6). We illustrate this process in detail below.

First, let us apply the stationary phase result of (2.5) to the integrals in (2.11). Let us write $\Psi(yt, t) = I_{+1}(y, t) + I_{+2}(y, t) + I_{-1}(y, t) + I_{-2}(y, t) + R(t)$ where $R(t) = O(t^{-1})$ as $t \rightarrow \infty$, and where $I_{\pm 1}(y, t)$ is the contribution of the stationary phase point $\theta_{\pm 1}$ to the \pm subscripted integral, and likewise $I_{\pm 2}(y, t)$ is the corresponding contribution of $\theta_{\pm 2}$ to $I_{\pm 2}$. Directly applying (2.5),

$$I_{\pm 1}(y, t) = E_\pm(\theta_{\pm 1}) e^{it(\Xi_\pm(\theta_{\pm 1}) - y\theta_{\pm 1})} \sqrt{\frac{\pi}{t|\Xi''_\pm(\theta_{\pm 1})|}} (1 \pm i)$$

$$I_{\pm 2}(y, t) = E_\pm(\theta_{\pm 2}) e^{it(\Xi_\pm(\theta_{\pm 2}) - y\theta_{\pm 2})} \sqrt{\frac{\pi}{t|\Xi''_\pm(\theta_{\pm 2})|}} (1 \pm i).$$

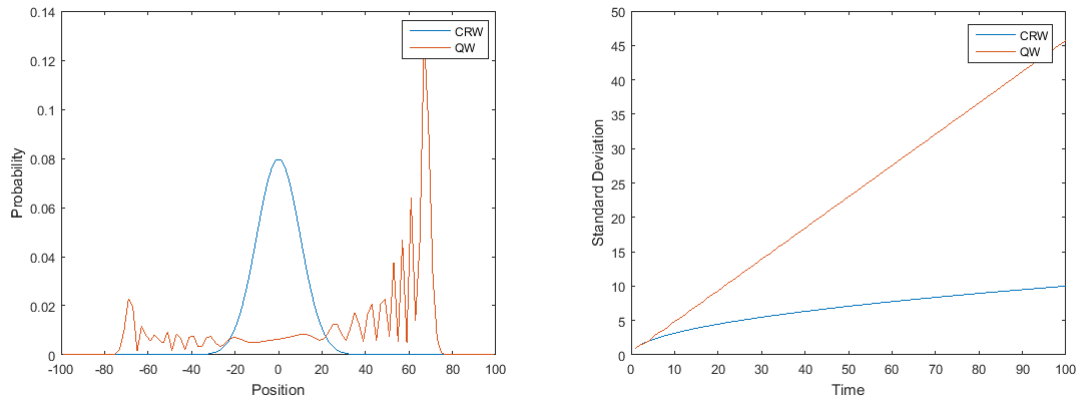


Figure 2.1: (*Left*) Probability distribution of the (\mathbb{Z}, C_1, H) Hadamard walk initialized at $|0\rangle|R\rangle$ and classical random walk after 100 iterations (*Right*) Plot of standard deviation vs time for both the (\mathbb{Z}, C_1, H) Hadamard walk and classical random walk.

The result follows directly from substituting the equations from Lemmas 2.4 through 2.6 into these $I(y, t)$ functions and taking a sum. \square

The theorem explicitly summarizes the linear spreading of this one dimensional quantum walk. The oscillatory components $\text{Re} \left[E e^{i\pi/4} \frac{g(y)^t}{f(y)^{yt}} \right]$ of the state representation from the theorem tell us that the probability distribution is highly oscillatory toward the edges of the region of polynomial decay, while it is nearly uniform in a neighborhood of the origin. Further, the term $\sqrt{\frac{\pi|b|}{t(1-y^2)\sqrt{|a|^2-y^2}}}$ indicates that the distribution approaches a singularity toward the edges of the region of polynomial decay. The term $(1 + (-1)^{t(y+1)})$ represents the parity of the quantum walk; that is, for a state initialized at $|0\rangle$, the amplitudes are non-vanishing only at odd positions when t is odd, and are non-vanishing only at even positions when t is even.

Localization Phenomena: The Grover Walk

We now illustrate how localization arises in the one-dimensional three state $(\mathbb{Z}, \tilde{C}_1, G_3)$ Grover walk [37]. This is a phenomenon permitted at isolated values of y such as the origin in the asymptotic expansion of the quantum walk; see Theorem 2.3 below. Here,

$G_3 = \frac{1}{3} \begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}$ and $\tilde{C}_1 = \{1, 0, -1\} = \{R, S, L\}$. Note that in this case we have three states at each location $x \in \mathbb{Z}$, with particles in the $|R\rangle$ and $|L\rangle$ states moving left and right after applying the translation operator, while a particle in the $|S\rangle$ state does not move at all in a transition.

An extraordinary property of such walks (as well as some others) is that of *localization*, in which the time average of the walker's probability distribution limits to a nonzero value at the initial position.

We first consider the eigenvalues of the multiplier matrix. Let $M(\theta) = \begin{bmatrix} e^{i\theta} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & e^{-i\theta} \end{bmatrix} G_3$ be the Fourier multiplier matrix associated with the three state Grover walk. ASdirect calculation shows that the eigenvalues of this multiplier matrix satisfy the characteristic equation:

$$(\lambda(\theta) - 1) \left(\lambda(\theta)^2 + \frac{2}{3}(\cos \theta + 2) \lambda(\theta) + 1 \right) = 0. \quad (2.21)$$

Let the roots be indexed as $\lambda_{\pm}(\theta) = \frac{1}{3} \left[-(2 + \cos \theta) \pm i \sqrt{(5 + \cos \theta)(1 - \cos \theta)} \right]$, and $\lambda_0 = 1$. The eigenvalues $\lambda_{\pm}(\theta)$ share a similar structure to those arising from the unitary (\mathbb{Z}, C_1, U) quantum walk on the integers, and it has been shown [27] that computing the same inverse Fourier transforms as in the previous section for the now three state amplitudes $\Psi(x, t)$ leads to highly ballistic behavior that is similar to the general two-state quantum walk. Given our general theorem (Theorem 2.3 below), this walk applies directly and it remains to determine the region of polynomial decay. Recall that from Definition 2.3, the region of polynomial decay associated with an eigenvalue $\lambda(\theta) = e^{i\Xi(\theta)}$ of the Fourier multiplier matrix $M(\theta)$ is the set $\Xi'[-\pi, \pi]$. By writing out the function $\Xi'(\theta)$ as

in equation (2.7), we have

$$\Xi'(\theta) = \frac{\sin \theta}{\sqrt{9 - (\cos \theta + 2)^2}}$$

By using a simple calculus argument to determine the minimum and maximum of $\Xi'(\theta)$, we arrive at the following proposition:

Proposition 2.5 *The region of polynomial decay associated to each of the nonconstant eigenvalues of the one-dimensional three-state Grover matrix is the interval $\left[-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\right]$.*

This result also follows from work of Falkner et. al. on the Grover walk; see [27]. To illustrate specifically the phenomenon of localization we note that the constant eigenvalue $\lambda_0 = 1$ causes localization at the origin, i.e. an exceptional point (see Theorem 2.3 below) at which the solution does not decay. For almost every compactly supported initial condition Ψ_0 , the three state Grover walk has a solution $\Psi(yt, t)$ that decays superpolynomially for $|y| > \frac{1}{\sqrt{3}}$ and polynomially for $|y| \leq \frac{1}{\sqrt{3}}$, if $y \neq 0$. More specifically, in the first region $|\Psi(yt, t)| < t^{-N}$ for all N as $t \rightarrow \infty$, while in the second region it behaves at each y as $C(y)t^{-1/2}$ as $t \rightarrow \infty$, i.e. it has precise order $\Theta(t^{-1/2})$.

The eigenvalue $\lambda_0 = 1$ causes a breakdown of the stationary phase approximation in (2.5) which leads to localization. Let $E_0(\theta)$ and $E_{\pm}(\theta)$, the eigenvectors corresponding to λ_0 and λ_{\pm} respectively, be normalized as above so that (2.3) solves our initial value problem $\Psi(x, 0) = \Psi_0 = |0\rangle(\alpha|R\rangle + \beta|S\rangle + \gamma|L\rangle)$. We may now represent $\Psi(yt, t)$ according to (2.3) as:

$$\begin{aligned} \Psi(yt, t) &= \frac{1}{2\pi} \int_{-\pi}^{\pi} E_0(\theta) e^{it(\Xi_0(\theta) - y\theta)} d\theta + \frac{1}{2\pi} \int_{-\pi}^{\pi} E_+(\theta) e^{it(\Xi_+(\theta) - y\theta)} d\theta \\ &\quad + \frac{1}{2\pi} \int_{-\pi}^{\pi} E_-(\theta) e^{it(\Xi_-(\theta) - y\theta)} d\theta. \end{aligned}$$

Let $I(y, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} E_0(\theta) e^{it(\Xi_0(\theta) - y\theta)} d\theta$. Since $\Xi_0(\theta) = 0$,

$$I(y, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} E_0(\theta) e^{-ity\theta} d\theta.$$

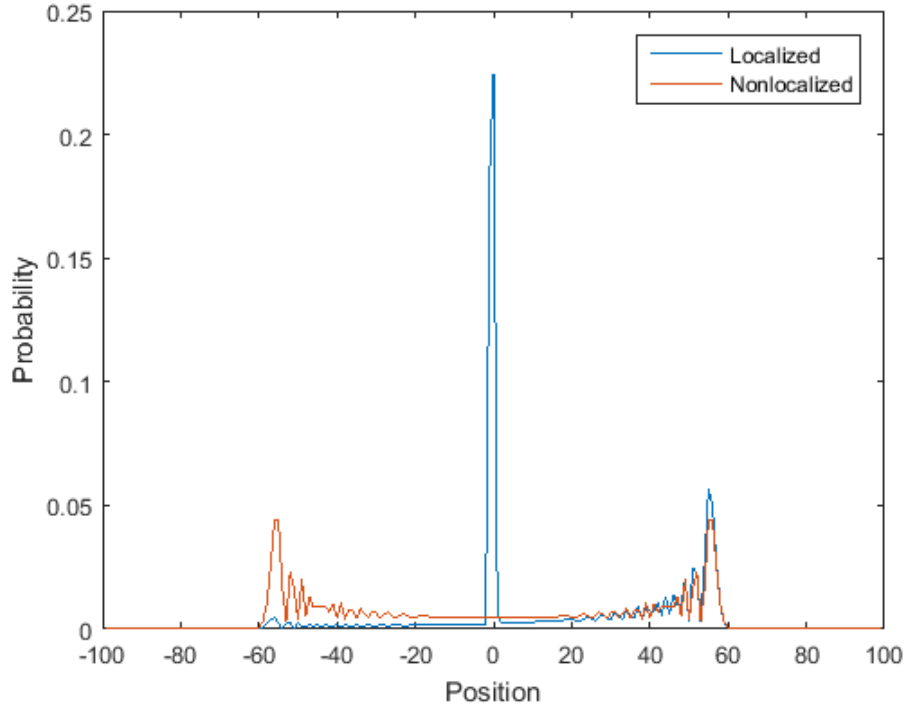


Figure 2.2: Comparison of probability distributions of Grover walks for initial conditions $|0\rangle|R\rangle$ (*blue*) and $\frac{1}{\sqrt{6}}|0\rangle(|R\rangle - 2|S\rangle + |L\rangle)$ (*red*)

If $y \neq 0$, then this integral decays superpolynomially in time. Thus, we approximate $I(y, t)$ at $y = 0$ and find the following. Setting $y = 0$ gives

$$I(0, t) = \frac{1}{2\pi} \int_{-\pi}^{\pi} E_0(\theta) d\theta.$$

This component of the solution is independent of time and gives the explicit amplitude of the Grover walk at the origin. However, as this integral is dependent on $E_0(\theta)$, localization does not necessarily occur for all initial conditions. Specifically, we find that for initial conditions with $\alpha = \gamma = \frac{1}{\sqrt{6}}$ and $\beta = \frac{2}{\sqrt{6}}$ there is an absence of localization, as illustrated in Figure 2 (See discussion after Theorem 2.3).

Revisiting Theorem 2.1

We can generalize Theorem 2.1 to a precise statement answering Conjecture 1.1 affirmatively in one dimension.

Below we denote L_1, \dots, L_n to be the set of states at a given point.

Theorem 2.3 *Consider a one dimensional quantum walk with n states with corresponding translations $\{\sigma_1, \dots, \sigma_n\}$ and a Fourier transform matrix*

$$M(\theta) = \begin{bmatrix} e^{i\sigma_1\theta} & 0 & \dots & 0 \\ 0 & e^{i\sigma_2\theta} & \dots & \vdots \\ \vdots & & \ddots & 0 \\ 0 & \dots & 0 & e^{i\sigma_n\theta} \end{bmatrix} U$$

(note θ here is a scalar) with U a fixed $n \times n$ unitary matrix, and an initial state $\Psi_0 = \sum_{j=1}^J |j\rangle (\alpha_{j1}|\sigma_1\rangle + \dots + \alpha_{jn}|\sigma_n\rangle)$ that is compactly supported. Then the subsequent states $\Psi(x, t) = \mathcal{F}^{-1} [M(\theta)^t \mathcal{F}[\Psi_0]]$ have the following characterization.

(a) *There is a set S such that if $y \notin S$, the amplitude $|\Psi(yt, t)|$ has superpolynomial decay (i.e. $O(t^{-N})$ for all $N > 0$) independently of initial condition.*

(b) *For all but a finite set of $y \in S$, and all compactly supported initial conditions $\Psi_0 \in \ell^2(\mathbb{Z}) \otimes \{L_1, \dots, L_n\}$ except for a set of measure 0, the amplitude has decay of order $-1/2$ (i.e. is of precise order $\Theta(t^{-1/2})$).*

Proof: As above, we write

$$\Psi(x, t) = (M(\theta)U)^t \Psi_0 = \frac{1}{2\pi} \sum_{j=1}^n \int_{|\theta| \leq \pi} E_j(\theta) e^{it(\Xi_j(\theta) - y\theta)} d\theta, \quad (2)$$

where the coefficients $E_j(\theta) (= v_j(\theta) \cdot \widehat{\Psi}_0(\theta))$, where $v_j(\theta)$ are normalized eigenvectors of $M(\theta)$ chosen so as to be analytic [Kato, Section II.3.3 [39]] and $\widehat{\Psi}_0(\theta)$ is the Fourier transform of the initial condition $\Psi(x, 0)$.

Let $S = \bigcup_{j=1}^n \Xi'_j([- \pi, \pi])$; note that S is bounded since $\Xi'(\theta)$ is analytic.

First, if $y \notin \Xi'_j([-\pi, \pi])$ for any j , then the exponents $\Xi_j(\theta) - y\theta$ have no points θ for which the derivative vanishes, and so by Proposition 2.1, the function $\Psi(yt, t)$ has superpolynomial decay. This proves (a).

To prove (b), we require the stationary phase approximation above. We fix $y \in \mathbb{R}$.

For each integral in (2), we use equation (2.5) to write just the first order stationary phase contributions to $\Psi(x, t)$ at the points θ_{jk} , where $\{\theta_{jk}\}_k$ is the listing of the (finite number of) points satisfying $\frac{d}{d\theta}\Xi_j(\theta) - y = 0$, or $\Xi'_j(\theta_{jk}) = y$ for all k .

We first consider the case that for given $y \in S$ there is a θ_{jk} for which $\Xi''(\theta_{jk}) = 0$. We will show first that there is a finite number of such y . Indeed, if there were an infinite collection Y_1 of such y , then there would be a single j (without loss assume it is $j = 1$) for which there is an infinite collection of y and values $\theta_{1k}(y)$ such that $\Xi'_1(\theta_{1k}(y)) = y$ and $\Xi''_1(\theta_{1k}) = 0$. Again without loss assume that for an infinite number of y we have that $\Xi'(\theta_{11}(y)) = y$ and $\Xi''(\theta_{11}(y)) = 0$. We then see that since $\theta_{11}(y)$ is continuous, if y takes on a set of values with an accumulation point, $\theta_{11}(y)$ will also have an accumulation point. However, since $\Xi''(\theta)$ is analytic, this means that $\Xi''(\theta) = 0$ everywhere. However, since $\Xi(\theta)$ is periodic, this implies that $\Xi(\theta) = 0$, which is impossible under our assumptions. Thus the set Y_1 of y for which there is a θ such that $\Xi'_j(\theta) = y$ and $\Xi''_j(\theta) = 0$, is finite.

Henceforth we assume that $y \notin Y_1$. Then we can use the method of stationary phase (equation (2.5)) to conclude that

$$\begin{aligned} \Psi(yt, t) &= \frac{1}{\sqrt{t}} \sum_{j=1}^n \sum_k E_j(\theta_{jk}) e^{it(\Xi_j(\theta_{jk}) - y)} \sqrt{\frac{\pi}{\Xi''_j(\theta_{jk})}} + O(t^{-1}) \\ &= \frac{1}{\sqrt{t}} T(y) + O(t^{-1}), \end{aligned} \quad (2)$$

where we define

$$T(y) = \sum_{j=1}^n \sum_k E_j(\theta_{jk}) e^{it(\Xi_j(\theta_{jk}) - y)} \sqrt{\frac{\pi}{\Xi''_j(\theta_{jk})}}. \quad (3)$$

Thus unless there are cancellations in the sum (3) so that it vanishes, the function $\Psi(ty, y)$ above behaves asymptotically as $T(y)/\sqrt{t}$.

However, we claim that the sum $T(y)$ can vanish for at most a finite number of $y \in S$. To this end, note that above $\theta_{jk} = \theta_{jk}(y)$. Assume for a contradiction that there is an infinite collection Y_2 of y such that $T(y)$ vanishes, and hence that such y form a set with an accumulation point y^* . We will show that $T(y)$ is an analytic function of y with at most a finite number of branch points, so that (3) would vanish everywhere if the set Y_2 had an accumulation point, which would give a contradiction.

To show the above claim that $T(y)$ on S is analytic in y with at most a finite number of branch points, we need to show the the exponents $\Xi_j(\theta_{jk}) - y = \Xi_j(\theta_{jk}(y)) - y$ have this property, i.e. are analytic in y with finitely many branch points. Since Ξ_j are analytic functions, it suffices to show that the same is true of the functions $\theta_{jk}(y)$. Note $\theta_{jk}(y)$ solves $\Xi'_j(\theta_{jk}(y)) = y$, i.e., $\theta_{jk}(y) = \Xi_j^{-1}(y)$. Since the function $\Xi'_j(\theta)$ is analytic on a bounded domain and into a bounded range, the inverse $(\partial_y \Xi_j)^{-1}(y)$ is also analytic outside of finitely many (or no) branch points. To see there are no more than a finite number of branch points, note that any such point in the inverse function $(\partial_y \Xi_j)^{-1}(y)$ would occur at a value of $\theta = \Xi_j^{-1}(y)$ such that $\Xi''(\theta) = 0$. Since there are a finite number of such θ , there are a finite number of branch points. Thus also $T(y)$ has at most finitely many branch points and is otherwise analytic.

For this reason the set Y_2 is also finite. For y outside the finite set $Y_1 \cup Y_2 \subset S$, the behavior of $\Psi(ty, t)$ for $y \in S$ is of the form (2), with $T(y) \neq 0$.

We must consider the separate case in which one or more eigenvalues $\lambda_j(\theta)$ are constant. In this case we have $\Xi_j(\theta) \equiv 0$, and from equation (2) we see that (given that $E_j(\theta)$ is either constant or analytic for all θ , including $\theta = \pm\pi$) for $y \neq 0$ we have exponential decay in the integral $\int_{|\theta| \leq \pi} E_j(\theta) e^{it(\Xi_j(\theta) - y\theta)} d\theta$ that forms the j^{th} term of the sum (note $\Xi_j \equiv 0$ here). However for $y = 0$ this integral is independent of t , and so generally fails to go to 0. In such cases the point $y = 0$ therefore counts among the finite number of points in S for which the $O(1/\sqrt{t})$ dependence fails.

Finally, we show that the above holds for almost every initial condition $\Psi_0(x, t)$ that is compactly supported. First note that the statement that this holds for almost every initial condition means that among all $\Psi_0(x, t)$ supported in a fixed compact set (which forms a finite dimensional set), the set of such $\Psi_0(x, t)$ for which the above statement fails has measure 0. Indeed, the statement fails only for those $\widehat{\Psi}_0(x, t)$ for which the Fourier transform $\widehat{\Psi}_0(\theta, t)$ forces one of the terms

$$E_j(\theta_{jk})e^{it(\Xi_j(\theta_{jk})-y)}\sqrt{\frac{\pi}{\Xi_j''(\theta_{jk})}} = v_j(\theta_{jk}) \cdot \widehat{\Psi}_0(\theta_{jk})e^{it(\Xi_j(\theta_{jk})-y)}\sqrt{\frac{\pi}{\Xi_j''(\theta_{jk})}}$$

in the above sum (3) to vanish. This can only occur when the inner product $v_j(\theta_{jk}) \cdot \widehat{\Psi}_0(\theta_{jk})$ vanishes, which can clearly only occur for a set of $\widehat{\Psi}_0(\theta_{jk})$ of measure 0.

This completes the proof. \square

Remark: We note that the last case (of constant eigenvalues) leads to so-called localization phenomena, which are illustrated in more detail for the Grover walk below. In such cases, typically, we have a non-diminishing positive probability of recurrence at the origin for all time. This is a phenomenon that is not seen in the classical walk, in which probability of recurrence at the origin decays as $1/\sqrt{t}$.

2.4 Regions of Polynomial Decay in Two Dimensional Walks

In this section, we apply the stationary phase analysis to analyze several two dimensional quantum walks. In these cases, we will be less interested in precise asymptotic expansions and more so in computing regions of polynomial decay that are analogs of the same regions in one dimension (as in Theorem 2.1). The coin operator U at each point $x \in \mathbb{Z}^2$ is unchanged, and can take the same forms as in one dimension. The Fourier multiplier matrix $M(\theta_1, \theta_2) = \text{diag} [e^{i\sigma_1 \cdot \theta_1}, \dots, e^{i\sigma_n \cdot \theta_n}]$ corresponding to a quantum walk operator on \mathbb{Z}^2 is now dependent on two transform variables θ_1 and θ_2 . As mentioned previously, if $\lambda(\theta_1, \theta_2) = e^{i\Xi(\theta_1, \theta_2)}$ is an eigenvalue of $M(\theta_1, \theta_2)$, then a parametric description of the

region of polynomial decay is given by $(\nabla \Xi)([-\pi, \pi]^2)$ where $[-\pi, \pi]^2$ is the domain of integration in the inverse Fourier transform. In the two dimensional Grover (\mathbb{Z}^2, C_2, G_4) quantum walk, after factoring out the constant eigenvalues, the nonconstant eigenvalues $\lambda(\theta_1, \theta_2)$ of $M(\theta_1, \theta_2)$ satisfy a quadratic equation of the form:

$$\lambda(\theta_1, \theta_2)^2 + 2a(\theta_1, \theta_2)\lambda(\theta_1, \theta_2) + 1 = 0$$

where $a(\theta_1, \theta_2)$ is an analytic function (we do not specify this function at the moment since this calculation will be a model for further calculations later on). We can proceed as in the previous section to find:

$$\nabla \Xi = \pm \left(\frac{a_{\theta_1}}{\sqrt{1-a^2}}, \frac{a_{\theta_2}}{\sqrt{1-a^2}} \right).$$

where $a = a(\theta_1, \theta_2)$ and $a_{\theta_1} = \frac{\partial a}{\partial \theta_1}(\theta_1, \theta_2)$.

For future reference we will here consider some examples that will occur later for which the nonconstant eigenvalues $\lambda(\theta_1, \theta_2)$ will satisfy a special quartic equation:

$$\lambda^4 + x\lambda^3 + y\lambda^2 + x\lambda + 1 = 0. \tag{B}$$

Here, $x = x(\theta_1, \theta_2)$ and $y = y(\theta_1, \theta_2)$. We note for later use that such quartic polynomials can be factored as:

$$(\lambda^2 + a\lambda + 1)(\lambda^2 + b\lambda + 1) = 0$$

where

$$a + b = x, \quad ab + 2 = y. \tag{2.22}$$

In such situations, finding $\nabla \Xi$ via multiple applications of the chain rule can be very difficult and unintuitive, so that we will choose implicit differentiation. Our goal will be to express $\nabla \Xi$ in terms of x , y , and their derivatives. Suppose an eigenvalue satisfies $\lambda^2 + a\lambda + 1 = 0$.

Using the one dimensional results from the previous section, we have $\Xi_{\theta_1} = -\frac{a_{\theta_1}}{i(2\lambda+a)}$, and likewise for a derivative in θ_2 . Upon differentiating the system relating (a, b) to (x, y) , we may represent the derivative a_{θ_1} as:

$$a_{\theta_1} = \frac{ax_{\theta_1} - y_{\theta_1}}{2a - x}.$$

A similar equation holds for derivatives with respect to θ_2 . We can solve equations (2.16) to show that $a = \frac{1}{2} \left[x \pm \sqrt{x^2 - 4y + 8} \right]$, and thus:

$$\Xi_{\theta_1} = \pm \frac{ax_{\theta_1} - y_{\theta_1}}{\sqrt{(x^2 - 4y + 8)(4 - a^2)}}, \quad (2.23)$$

with a similar formula for Ξ_{θ_2} . This yields a formula for $\nabla\Xi(\theta_1, \theta_2)$ that allows computation of the range $S = \nabla\Xi([-\pi, \pi]^2)$ of the gradient of Ξ .

As done earlier, using the methods of Theorem 2.2, if we find that the eigenvalues $\lambda(\theta)$ are analytic functions on $\theta \in [-\pi, \pi]^2$, we can show that, except on a set of y -measure 0 (where individual terms in the stationary phase expansion might cancel), there will be polynomial decay of $\Psi(yt, t)$ for $y \in \nabla\Xi([-\pi, \pi]^2)$ (i.e. it will behave asymptotically as $y^{-\delta}$, with $\delta \geq 0$). This parametric description of the regions of polynomial decay provided by computation of $\nabla\Xi$ in equations such as (2.17) is useful for computing contour plots for the region of polynomial decay, but not for succinctly describing such regions. However, in certain cases, we will find that $\nabla\Xi$ is a vector valued algebraic function of $\cos \theta_1$ and $\cos \theta_2$. This will allow us to describe the region directly in the form of an inequality $F(X, Y) \geq 0$, where X and Y are coordinates in \mathbb{R}^2 and F is a polynomial in X and Y . In practice this is difficult for multi-dimensional walks unless the characteristic polynomial of the associated multiplier matrix can be sufficiently factored.

Displaying Numerical Simulations of Two Dimensional Quantum Walks

In the coming sections we will display figures comparing a numerical simulation and a contour plot of the regions of polynomial decay for each quantum walk discussed. We choose to display the numerical simulations as two dimensional density plots where the images are saturated to highlight internal structure. The white portions of the images correspond to regions of higher probability. However, these images would be rendered useless for quantum walks with localization as only the origin would appear bright and the rest of the probability distribution would be comparatively dark. In these cases, we choose a specific initial condition to remove localization as we illustrated in the case of the $(\mathbb{Z}, \tilde{C}_1, G_3)$ quantum walk in Figure 2.2.

Example: Two Dimensional (\mathbb{Z}^2, C_2, G_4) Grover Walk

As our first example, we consider the two dimensional four-state Grover walk (\mathbb{Z}^2, C_2, G_4)

[36]. Here, $C_2 = \{(1, 0), (-1, 0), (0, 1), (0, -1)\}$ and $G_4 = \frac{1}{2} \begin{bmatrix} -1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 \\ 1 & 1 & -1 & 1 \\ 1 & 1 & 1 & -1 \end{bmatrix}$. This im-

plies the multiplier matrix of this quantum walk operator may be written as $M(\theta_1, \theta_2) =$

$\begin{bmatrix} e^{i\theta_1} & 0 & 0 & 0 \\ 0 & e^{-i\theta_1} & 0 & 0 \\ 0 & 0 & e^{i\theta_2} & 0 \\ 0 & 0 & 0 & e^{-i\theta_2} \end{bmatrix} G_4$. This walk is a primary example of a two dimensional quantum walks studied in the literature ([36], [68], [47]).

We first compute the characteristic polynomial of the corresponding multiplier matrix. If $M(\theta_1, \theta_2)$ is the multiplier matrix corresponding to the two dimensional four-state Grover walk, the eigenvalues $\lambda(\theta_1, \theta_2)$ satisfy:

$$(\lambda^2 - 1)(\lambda^2 + (\cos \theta_1 + \cos \theta_2)\lambda + 1) = 0 \quad (2.24)$$

From our earlier discussion regarding constant eigenvalues, it is clear that the eigenvalues $\lambda = \pm 1$ contribute to the localization of this walk. The remaining two eigenvalues can be written as

$$\lambda_{\pm}(\theta_1, \theta_2) = \frac{1}{2} \left[-(\cos \theta_1 + \cos \theta_2) \pm i\sqrt{4 - (\cos \theta_1 + \cos \theta_2)^2} \right].$$

We now prove the following result describing the region of polynomial decay corresponding to these eigenvalues.

Proposition 2.6 *For both eigenvalues $\lambda_{\pm}(\theta_1, \theta_2)$, the corresponding regions $S_{\pm} = \nabla\Xi([- \pi, \pi]^2)$ of polynomial decay in variables $(X, Y) \in \mathbb{R}^2$ consists of the region:*

$$\frac{1}{2} - X^2 - Y^2 > 0 \tag{2.25}$$

Proof: To find the described regions of polynomial decay, we write $\nabla\Xi_{\pm}(\theta_1, \theta_2) = (X, Y)$.

We can use the results from (2.17) to write:

$$X = \mp \frac{\sin \theta_1}{\sqrt{4 - (\cos \theta_1 + \cos \theta_2)^2}}, \quad Y = \mp \frac{\sin \theta_2}{\sqrt{4 - (\cos \theta_1 + \cos \theta_2)^2}}. \tag{2.26}$$

We can solve for $\cos \theta_2$ in terms of X and $\cos \theta_1$ as follows:

$$\cos \theta_2 = -\cos \theta_1 \pm \frac{\sqrt{4X^2 + \cos^2 \theta_1 - 1}}{X}.$$

Since we have divided by X , let us assume $X \neq 0$ and also $\sin \theta_1 \neq 0$. By substituting this expression for $\cos \theta_2$ into the right side of the second equation of (2.20), we can rearrange terms to arrive at a quadratic equation in $\cos^2 \theta_1$ with coefficients in X and Y . Let $A = 1 - 3X^2 - Y^2$ and $B = Y^2 - X^2 - 1$ such that the aforementioned quadratic equation becomes:

$$A^2 + (2AB - 4X^2(4X^2 - 1)) \cos^2 \theta_1 + (B^2 - 4X^2) \cos^4 \theta_1 = 0.$$

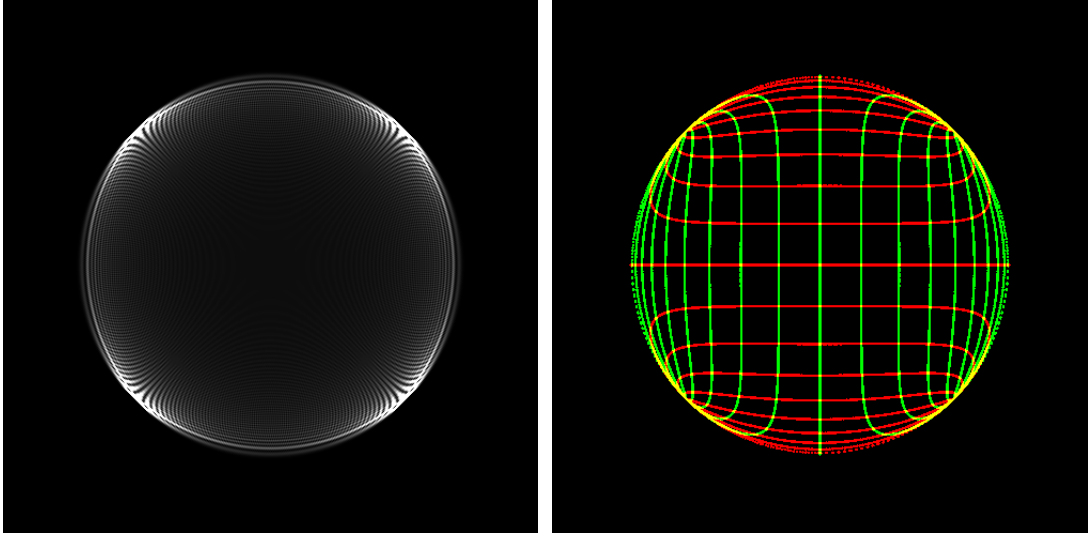


Figure 2.3: (*Left*) Simulation of (\mathbb{Z}^2, C_2, G_4) quantum walk with initial condition which eliminates localization (*Right*) Contour plot of the region of polynomial decay

This polynomial may be factored to give:

$$\sin^2 \theta_1 ((B^2 - 4X^2) \cos^2 \theta_1 - A^2) = 0.$$

Since $\sin^2 \theta_1 \neq 0$, we must have $\cos^2 \theta_1 = \frac{A^2}{B^2 - 4X^2}$. Recognizing that $\cos^2 \theta_1 < 1$, we can rearrange terms in this equation to arrive at the result off of the line $X = 0$. To complete the proof, simply set $X = 0$ such that $\theta_1 = 0$, and solve the second part of (2.20) in terms of Y . □

$(\mathbb{Z}^2, \tilde{C}_2, G_5)$ Quantum Walk

If we adjoin an additional internal state to the previous two dimensional four state Grover walk, we find that the regions of polynomial decay are altered. In this example, we consider

the $(\mathbb{Z}^2, \tilde{C}_2, G_5)$ quantum walk where $\tilde{C}_2 = C_2 \cup \{(0, 0)\}$ and G_5 is represented as:

$$G_5 = \frac{1}{5} \begin{bmatrix} -3 & 2 & 2 & 2 & 2 \\ 2 & -3 & 2 & 2 & 2 \\ 2 & 2 & -3 & 2 & 2 \\ 2 & 2 & 2 & -3 & 2 \\ 2 & 2 & 2 & 2 & -3 \end{bmatrix} \quad (2.27)$$

This walk was first introduced by Ampadu [10] in which localization was the main focus.

If $M(\theta_1, \theta_2)$ is the multiplier matrix corresponding to the two dimensional five-state Grover walk, then we may write this matrix as:

$$M(\theta_1, \theta_2) = \begin{bmatrix} e^{i\theta_1} & 0 & 0 & 0 & 0 \\ 0 & e^{-i\theta_1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & e^{i\theta_2} & 0 \\ 0 & 0 & 0 & 0 & e^{-i\theta_2} \end{bmatrix} G_5.$$

The eigenvalues $\lambda(\theta_1, \theta_2)$ of $M(\theta_1, \theta_2)$ satisfy the equation:

$$(\lambda - 1)\left(\lambda^4 + \frac{2}{5}(3c_1 + 3c_2 + 4)\lambda^3 + \frac{2}{5}(4c_1 + 4c_2 + 2c_1c_2 + 5)\lambda^2 + \frac{2}{5}(3c_1 + 3c_2 + 4)\lambda + 1\right) = 0 \quad (2.28)$$

Here, $c_1 = \cos \theta_1$ and $c_2 = \cos \theta_2$. The eigenvalue $\lambda = 1$ indicates that localization is present in this Grover walk. This characteristic polynomial has the form of equation (B) so the contours may be solved for as dictated by formula (2.17) from the beginning of this section.

Proposition 2.7 *The nonlocalized regions of polynomial decay (regions of polynomial decay corresponding to nonconstant eigenvalues) for the $(\mathbb{Z}^2, \tilde{C}_2, G_5)$ quantum walk have pa-*

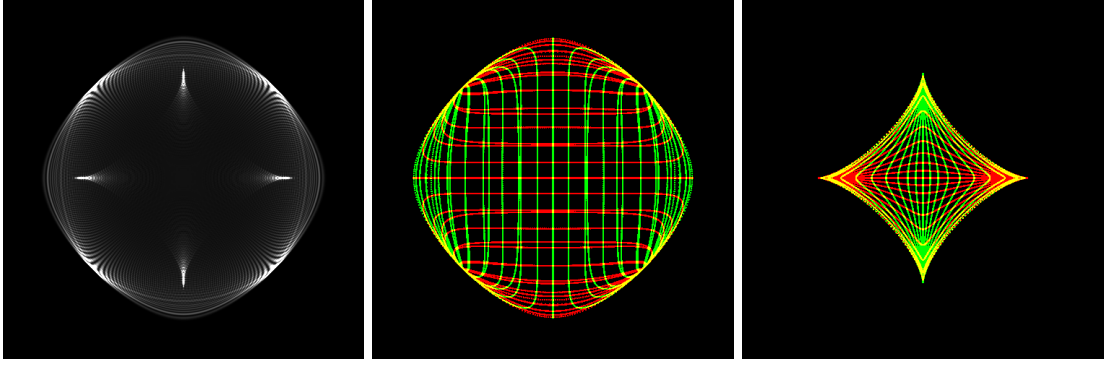


Figure 2.4: (*Left*) Simulation of $(\mathbb{Z}^2, \tilde{C}_2, G_5)$ quantum walk with initial condition which eliminates localization (*Right/Center*) Contour plots of two distinct regions of polynomial decay (initial conditions do not alter regions of polynomial decay) for the $(\mathbb{Z}^2, \tilde{C}_2, G_5)$ quantum walk.

parameterization

$$X(\theta_1, \theta_2) = \pm \frac{3a(\theta_1, \theta_2) \sin \theta_1 - 4 \sin \theta_1 - 2 \sin \theta_1 \cos \theta_2}{\sqrt{(9 \cos^2 \theta_1 + 9 \cos^2 \theta_2 - 2 \cos \theta_1 \cos \theta_2 - 16 \cos \theta_1 - 16 \cos \theta_2 + 16) (4 - a(\theta_1, \theta_2)^2)}} \quad (2.29)$$

$$Y(\theta_1, \theta_2) = \pm \frac{3a(\theta_1, \theta_2) \sin \theta_2 - 4 \sin \theta_2 - 2 \sin \theta_2 \cos \theta_1}{\sqrt{(9 \cos^2 \theta_1 + 9 \cos^2 \theta_2 - 2 \cos \theta_1 \cos \theta_2 - 16 \cos \theta_1 - 16 \cos \theta_2 + 16) (4 - a(\theta_1, \theta_2)^2)}} \quad (2.30)$$

where, if $c_1 := \cos \theta_1$ and $c_2 := \cos \theta_2$:

$$a(\theta_1, \theta_2) = \frac{1}{5} \left[3c_1 + 3c_2 + 4 \pm \sqrt{9c_1^2 + 9c_2^2 - 2c_1c_2 - 16c_1 - 16c_2 + 16} \right].$$

We display the contour plots in Figure 4. Unlike the other examples in this section, we find that the non-localized regions of polynomial decay for this quantum walk do not coincide.

Hexagonal Grover Walk

We now illustrate an example of a quantum walk which traverses a hexagonal lattice on \mathbb{Z}^2 as opposed to a rectangular lattice. The hexagonal or honeycomb lattice has been the subject of a few quantum walk investigations [1] [38] [48]. Define the set:

$$\begin{aligned}\Sigma &= \{(2, 0), (-1, 1), (-1, -1), (-2, 0), (1, -1), (1, 1)\} \\ &= \{R, LU, LD, L, RD, RU\}\end{aligned}\tag{2.31}$$

and consider the quantum walk $(\mathbb{Z}^2, \Sigma, U \otimes G_3)$ where $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ is an arbitrary 2×2 unitary matrix. If $a = 0$, then the amplitudes will travel on two separate hexagonal lattices. To be clear, this Hexagonal Grover Walk takes place on the subset of \mathbb{Z}^2 spanned by the elements of Σ . The value $|a|$ will determine the degree of mixing between the two lattices. For the remainder of this discussion, let $a = 0$ and $b = i$. We can write $M(\theta_1, \theta_2)$, the is the multiplier matrix corresponding to the hexagonal Grover walk, as:

$$M(\theta_1, \theta_2) = \begin{bmatrix} e^{2i\theta_1} & 0 & 0 & 0 & 0 & 0 \\ 0 & e^{i(-\theta_1+\theta_2)} & 0 & 0 & 0 & 0 \\ 0 & 0 & e^{-i(\theta_1+\theta_2)} & 0 & 0 & 0 \\ 0 & 0 & 0 & e^{-2i\theta_1} & 0 & 0 \\ 0 & 0 & 0 & 0 & e^{i(\theta_1-\theta_2)} & 0 \\ 0 & 0 & 0 & 0 & 0 & e^{i(\theta_1+\theta_2)} \end{bmatrix} \left(G_3 \otimes \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right).$$

The eigenvalues $\lambda(\theta_1, \theta_2)$ of $M(\theta_1, \theta_2)$ satisfy the equation:

$$(\lambda^2 - 1) \left(\lambda^4 - \frac{2}{9} [4 \cos 2\theta_2 + 8 \cos 3\theta_1 \cos \theta_2 - 3] \lambda^2 + 1 \right) = 0\tag{2.32}$$

Localization is present in the hexagonal Grover walk as indicated by the eigenvalues $\lambda = \pm 1$. The remaining four eigenvalues satisfy a quadratic equation in λ^2 . The equations

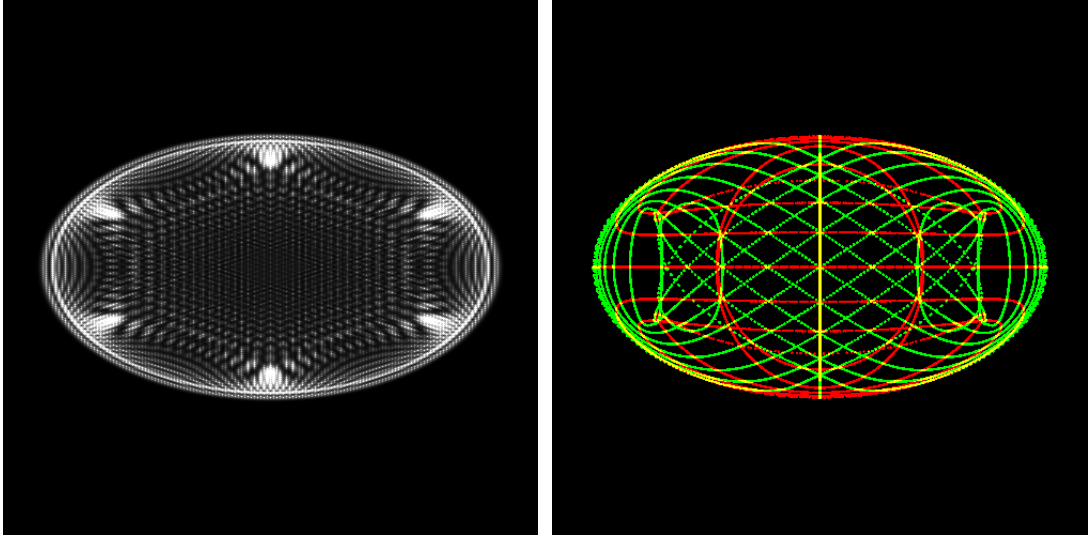


Figure 2.5: (*Left*) Simulation of the hexagonal Grover walk with initial condition which eliminates localization (*Right*) Contour plot of the region of polynomial decay for the hexagonal Grover walk.

at the beginning of the section may be altered to provide a parametric representation of the regions of polynomial decay, which we display below:

Proposition 2.8 *The non-localized regions of polynomial decay for the hexagonal Grover walk have parameterization*

$$X(\theta_1, \theta_2) = \pm \frac{4}{3} \frac{\sin 3\theta_1 \cos \theta_2}{\sqrt{81 - (4 \cos 2\theta_2 + 8 \cos 3\theta_1 \cos \theta_2 - 3)^2}} \quad (2.33)$$

$$Y(\theta_1, \theta_2) = \pm \frac{4}{9} \frac{\sin 2\theta_2 - \cos 3\theta_1 \sin \theta_2}{\sqrt{81 - (4 \cos 2\theta_2 + 8 \cos 3\theta_1 \cos \theta_2 - 3)^2}} \quad (2.34)$$

$(\mathbb{Z}^2, C_2, U_1 \otimes U_2)$ **Quantum Walk**

In this section, we consider a *tensor walk* which is represented as $(\mathbb{Z}^2, C_2, U_1 \otimes U_2)$ where $C_2 = \{(0, 1), (0, -1), (1, 0), (-1, 0)\}$, and $U_1 = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ and $U_2 = \begin{bmatrix} c & d \\ -\bar{d} & \bar{c} \end{bmatrix}$ are unitary matrices. A variant of this construction was considered by Baryshnikov et. al. [14]. The multiplier matrix $M(\theta_1, \theta_2)$ associated with this quantum walk operator may be written as:

$$M(\theta_1, \theta_2) = \begin{bmatrix} e^{i\theta_1} & 0 & 0 & 0 \\ 0 & e^{-i\theta_1} & 0 & 0 \\ 0 & 0 & e^{i\theta_2} & 0 \\ 0 & 0 & 0 & e^{-i\theta_2} \end{bmatrix} (U_1 \otimes U_2).$$

If $a, c \in \mathbb{R}$, then the eigenvalues $\lambda(\theta_1, \theta_2)$ of $M(\theta_1, \theta_2)$ satisfy the following equation:

$$\lambda^4 - 2ac(c_1 + c_2)\lambda^3 + (2c^2c_+ + 2(a^2 + c^2 - 1)c_- + 2a^2)\lambda^2 - 2ac(c_1 + c_2)\lambda + 1 = 0 \quad (2.35)$$

Here, $c_1 = \cos \theta_1$, $c_2 = \cos \theta_2$, and $c_{\pm} = \cos \theta_1 \pm \theta_2$. Notice here that the characteristic polynomial may be factored by using the argument at the beginning of the section. The case $a = c = \frac{1}{\sqrt{2}}$ is known as the Hadamard tensor walk. In this case the characteristic polynomial is simplified, but an algebraic representation of the regions of polynomial decay does not appear directly accessible. We display a parametric representation of these regions for the Hadamard tensor walk:

Proposition 2.9 *The regions of polynomial decay for the Hadamard tensor walk have parameterization*

$$X(\theta_1, \theta_2) = \pm \frac{a(\theta_1, \theta_2) \sin \theta_1 - \sin(\theta_1 + \theta_2)}{\sqrt{((\cos \theta_1 + \cos \theta_2)^2 - 4 \cos(\theta_1 + \theta_2) + 4) (4 - a(\theta_1, \theta_2)^2)}} \quad (2.36)$$

$$Y(\theta_1, \theta_2) = \pm \frac{a(\theta_1, \theta_2) \sin \theta_1 - \sin(\theta_1 + \theta_2)}{\sqrt{((\cos \theta_1 + \cos \theta_2)^2 - 4 \cos(\theta_1 + \theta_2) + 4) (4 - a(\theta_1, \theta_2)^2)}} \quad (2.37)$$

where $a(\theta_1, \theta_2) = \frac{1}{2} \left[-\cos \theta_1 - \cos \theta_2 \pm \sqrt{(\cos \theta_1 + \cos \theta_2)^2 - 4 \cos(\theta_1 + \theta_2) + 4} \right]$.

Based on the figures below, we are poised to make the following conjecture:

Conjecture 2.2 *Let S be a region of polynomial decay corresponding to an eigenvalue of the Hadamard tensor walk, and let us define the sets:*

$$S_{\pm} = \{(x, y) \in \mathbb{R}^2 : 6x^2 + 6y^2 - 4xy \pm 4(x - y) \leq 0\} \quad (2.38)$$

$$S_1 = \{(x, y) \in \mathbb{R}^2 : 1 - |x - y| - \sqrt{2}|x + y| \geq 0\}. \quad (2.39)$$

Then $(S_+ \cup S_- \cup S_1) \subset S$.

In this conjecture, S_{\pm} corresponds to the two ellipses and S_1 refers to the rhombus both visible at the top of Figure 2.6. We make this conjecture based on the numerical data available to us. There appears to be an interpolation between the minor axis of the rhombus and the two ellipses which is not accounted for by this conjecture.

2.5 Inhomogeneous Walks

The previous section focused on homogeneous quantum walks, or walks for which the quantum walk operator is spatially and temporally constant. We observed that these walks all exhibited linear spreading as described by Conjecture 1.1. We now shift our attention to inhomogeneous quantum walks, or quantum walks which use time and space dependent coins. In the examples that follow, we will find that periodic inhomogeneities in the quantum walk operator will lead to the familiar linear spreading of the previous sections. On the other hand, aperiodic inhomogeneities can lead to spreading of $O(\sqrt{t})$ as is typical of the classical random walk in time inhomogeneous quantum walks and Anderson localization in space inhomogeneous quantum walks.

Time Inhomogeneous Quantum Walk

We first introduce a definition for time inhomogeneous quantum walks:

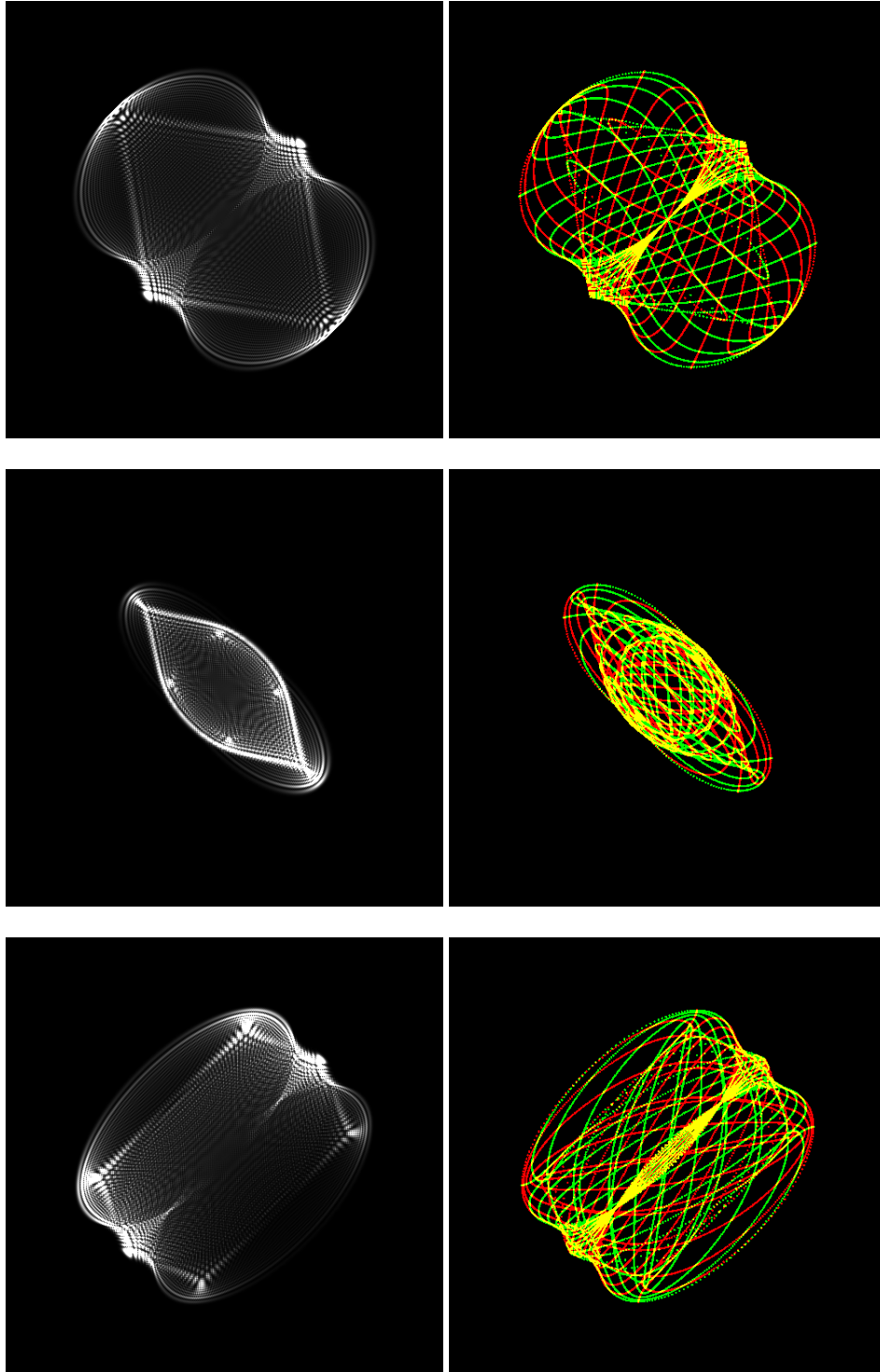


Figure 2.6: Numerical simulations and contour plots of regions of polynomial decay for $(\mathbb{Z}^2, C_2, U_1 \otimes U_2)$ tensor walks. (*Top*) $a = c = \frac{1}{\sqrt{2}}$ (*Center*) $a = \frac{3}{4}, c = \frac{1}{3}$ (*Bottom*) $a = \frac{2}{5}, c = \frac{8}{9}$

Definition 2.4 Let $Q_k \leftrightarrow (G, \Sigma, U_k)$ be a quantum walk operator for each $k = 1, 2, \dots$. We call the sequence $\{Q_1, Q_2, \dots\}$ a time inhomogeneous quantum walk. In particular, if the sequence $\{U_1, U_2, \dots\}$ is periodic with period p , we refer to the sequence of quantum walk operators as a periodic quantum walk with operator $Q = Q_p \dots Q_1$. Similarly if $\{U_1, U_2, \dots\}$ is aperiodic, we refer to the sequence of quantum walk operators as an aperiodic quantum walk.

Periodic quantum walks exhibit behavior similar to that of homogeneous quantum walks i.e. ones in which the coin operator U is constant. For example, let $\{Q_k\}$ be a periodic quantum walk with period p where $Q_k \leftrightarrow (\mathbb{Z}, C_1, U_k)$. If $Z = \begin{bmatrix} e^{i\theta} & 0 \\ 0 & e^{-i\theta} \end{bmatrix}$, then the multiplier matrix $M(\theta)$ of $Q(\theta) = Q_p \dots Q_1$ becomes the following:

$$M(\theta) = ZU_p ZU_{p-1} \dots ZU_1.$$

We consider a periodic quantum walk $\{Q_k\}$ of period 2 where $Q_k \leftrightarrow (\mathbb{Z}, C_1, U_k)$. Here, let $U_k = \begin{bmatrix} a_k & b_k \\ -\bar{b}_k & \bar{a}_k \end{bmatrix}$ be an arbitrary 2×2 unitary matrix. From the previous equation, we find the multiplier matrix becomes:

$$M(\theta) = \begin{bmatrix} a_1 a_2 e^{2i\theta} - \bar{b}_1 b_2 & b_1 a_2 e^{2i\theta} + \bar{a}_1 b_2 \\ -\bar{b}_1 \bar{a}_2 e^{-2i\theta} - a_1 \bar{b}_2 & \bar{a}_1 \bar{a}_2 e^{-2i\theta} - b_1 \bar{b}_2 \end{bmatrix}.$$

The eigenvalues $\lambda_{\pm}(\theta)$ of this matrix satisfy:

$$\lambda_{\pm}(\theta) = \text{Re} \left[a_1 a_2 e^{2i\theta} - \bar{b}_1 b_2 \right] \pm i \sqrt{1 - (\text{Re} \left[a_1 a_2 e^{2i\theta} - \bar{b}_1 b_2 \right])^2}.$$

Since $\lambda_{\pm}(\theta) = e^{i\Xi_{\pm}(\theta)}$, we can use previous equations to find:

$$\Xi'_{\pm}(\theta) = \mp \frac{2 \text{Im} (a_1 a_2 e^{2i\theta})}{\sqrt{1 - (\text{Re} \left[a_1 a_2 e^{2i\theta} - \bar{b}_1 b_2 \right])^2}}.$$

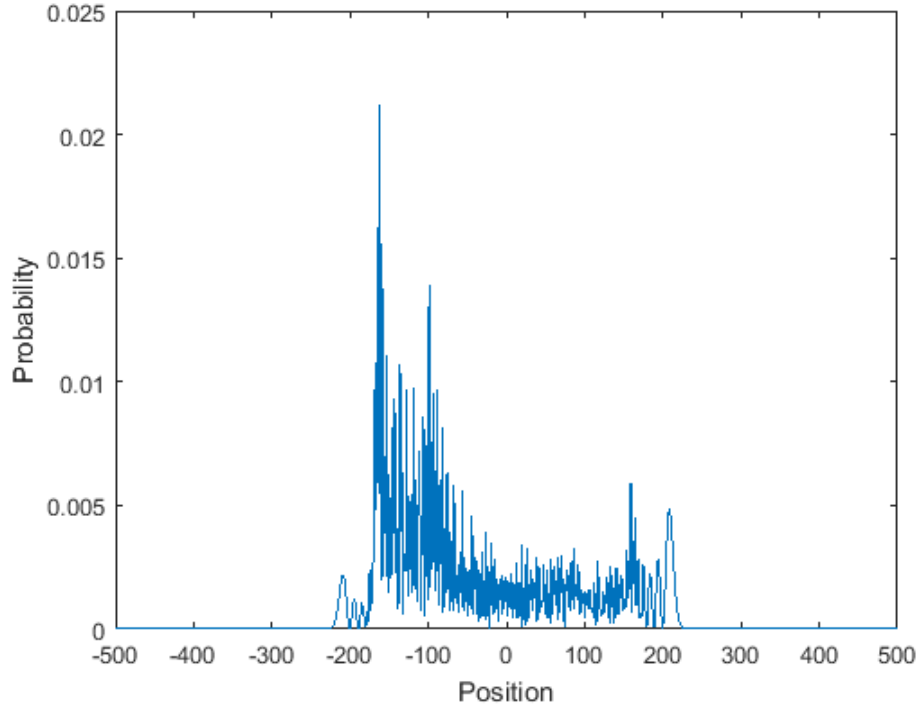


Figure 2.7: Typical probability distribution of a period 5 two state quantum walk (coins U_1, \dots, U_5 were randomly generated from a uniform distribution on the $|a|^2$ parameter

By finding the critical points, we see that $|\Xi'_\pm(\theta)|^2 \leq R(a_1, a_2, b_1, b_2)$ where R satisfies:

$$R(a_1, a_2, b_1, b_2) = \frac{4|a_1|^2|a_2|^2}{\operatorname{Re}(\bar{b}_1 b_2)x + 1 - (\operatorname{Re}(\bar{b}_1 b_2))^2}.$$

Here x satisfies the equation $\operatorname{Re}(\bar{b}_1 b_2)x^2 + (1 - (\operatorname{Re}(\bar{b}_1 b_2))^2 - |a_1|^2|a_2|^2)x + |a_1|^2|a_2|^2 \operatorname{Re}(\bar{b}_1 b_2) = 0$. Interestingly, R is independent of phase in a_1 or a_2 , and if $\operatorname{Re}(\bar{b}_1 b_2) = 0$, then $R(a_1, a_2, b_1, b_2) = 4|a_1|^2|a_2|^2$. This means that the region of polynomial decay for this period 2 quantum walk is the interval $(-|a_1||a_2|, |a_1||a_2|)$.

Aperiodic quantum walks resemble the classical random walk for large time [57]. These walks are difficult to analyze with the methods we are currently using, as no single multiplier matrix describes an aperiodic quantum walk in Fourier space. Several authors have opted to use probabilistic representations of the sequence $\{U_k\}$. Figures 7 and 8 below illustrate

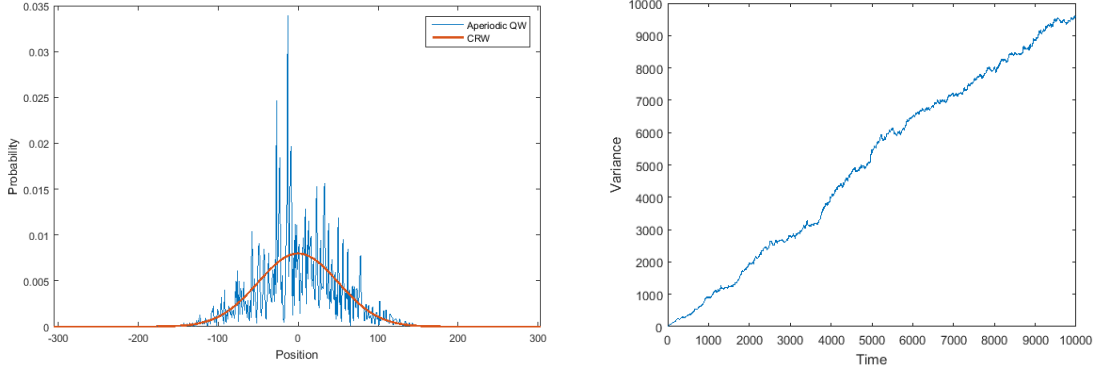


Figure 2.8: (*Left*) Probability distributions of aperiodic two state quantum walk (*blue*) and symmetric random walk (*red*). Here, the unitary coin at each time step is a general 2×2 unitary matrix U and we let $|a|^2$ be a uniform random variable. (*Right*) Plot of variance over time for a similar aperiodic two state quantum walk

typical probability distributions (squared amplitudes) of both periodic and aperiodic time-inhomogeneous quantum walks. Figure 8 also provides evidence that the variance of an aperiodic walk grows approximately linearly in time i.e. at a rate $O(t)$.

Electric Quantum Walk

The electric quantum walk [55] [20] is a special variant of a quantum walk with spatial inhomogeneity.

Definition 2.5 Let $Q \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ be a quantum walk operator with $Q = T(I \otimes U)$. We say that $Q_\Theta \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ is an electric quantum walk operator if $Q_\Theta = T(I \otimes e^{ix \cdot \Theta} U)$ where the unitary coin is space dependent and Θ is a fixed vector.

As with the time inhomogeneous quantum walk, there is a distinction between the periodic ($\Theta \in 2\pi\mathbb{Q}^d$) and aperiodic ($\Theta \notin 2\pi\mathbb{Q}^d$) cases of the electric quantum walk. Let us consider the electric quantum walk operator $Q_\Theta \leftrightarrow (\mathbb{Z}, C_1, U)$. Suppose $\Theta = 2\pi\frac{p}{q}$ where p and q have no common divisors. Let $S = \{r_1, l_1, \dots, r_q, l_q\}$ and let Z be a $q \times q$ diagonal matrix with $Z_{k,k} = e^{ik\Theta}$. If we adjust our translation operator T to act on the internal

states as:

$$T' : |x\rangle|r_k\rangle \mapsto |x\rangle|r_{k+1}\rangle, \quad (1 \leq k \leq q-1)$$

$$T' : |x\rangle|l_k\rangle \mapsto |x\rangle|l_{k-1}\rangle, \quad (2 \leq k \leq q) \quad (2.40)$$

$$T' : |x\rangle|r_q\rangle \mapsto |x+1\rangle|r_1\rangle, \quad T : |x\rangle|l_1\rangle \mapsto |x-1\rangle|l_q\rangle$$

then we find that Q_Θ is isomorphic to the modified quantum walk operator $Q = T'(I \otimes (Z \otimes U))$. The modified quantum walk operator Q essentially treats the collection of states $\{|n\rangle|\sigma\rangle : 1 \leq n \leq q, \sigma \in \{R, L\}\}$ of the typical one dimensional two state quantum walk as a collection of internal states in the modified quantum walk. This modified quantum walk operator is a homogeneous quantum walk operator (has a constant, position independent coin) and can thus be analyzed using the previous Fourier transform techniques.

In a similar manner to the previous section, we may construct a Fourier multiplier representation for the electric quantum walk which may be feasibly analyzed for $\theta \in 2\pi\mathbb{Q}$. Consider the electric quantum walk operator $Q_\theta \leftrightarrow (\mathbb{Z}, C_1, U)$ and let $\Psi : \mathbb{Z} \times \mathbb{N} \rightarrow \mathbb{C}^2$ be an amplitude function such that $\Psi(n, t) = [r(n, t), l(n, t)]'$ is the vector of amplitudes at position n and time t of the quantum walk. Then, these amplitude functions satisfy the following system of position dependent difference equations:

$$r(n, t+1) = ae^{i(n-1)\theta}r(n-1, t) + be^{i(n-1)\theta}l(n-1, t)$$

$$l(n, t+1) = -\bar{b}e^{i(n+1)\theta}r(n+1, t) + \bar{a}e^{i(n+1)\theta}l(n+1, t).$$

This system is very similar to the one referenced in the discussion of d -dimensional quantum walks, with a position dependent phase component included. Upon taking a Fourier transform of these difference equations, and letting $Z(k) = \begin{bmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{bmatrix}$, we arrive at:

$$\mathcal{F}[\Psi(n, t+1)](k) = Z(k)U\mathcal{F}[\Psi(n, t)](k + \theta).$$

We denote the Fourier transform variable here as k so that it is not confused with the electric quantum walk parameter Θ . If $\Theta = 2\pi\frac{p}{q}$, then the operator Q_θ^q has a corresponding Fourier multiplication matrix $M(k) = Z(k)UZ(k+\theta)U\dots Z(k+(q-1)\theta)U$. Since the electric quantum walk is isomorphic to a one dimensional quantum walk as defined by Definition 2.1, we can apply Theorem 2.1 to show that the electric quantum walk has a linearly expanding region of polynomial decay.

Cedzich et. al. [20] discuss three distinct cases of the electric quantum walk. By showing that an electric quantum walk with parameter $\theta = \frac{2\pi p}{q} \in 2\pi\mathbb{Q}$ is equivalent to a one-dimensional quantum walk with $2q$ internal spin states, we conclude that the amplitudes spread linearly. The the intermediate behavior of the electric quantum walk is very interesting especially for parameters with large denominators. The main result of the paper by Cedzich et. al. [20] is the revival theorem, which states:

Theorem 2.4 (Revival Theorem) *Let $\theta = 2\pi\frac{p}{q}$ where p and q have no common factors.*

If $Q_\theta \leftrightarrow (\mathbb{Z}, C_1, U)$ is an electric quantum walk operator with unitary matrix $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$,

then the following norm equalities hold:

$$\|Q_\theta^{2q} + I\|_{op} = 2|a|^q, \quad q \text{ odd}$$

$$\|Q_\theta^q + (-1)^{m/2}I\|_{op} = 2|a|^{q/2}, \quad q \text{ even.} \quad (2.41)$$

The proof of this theorem hinges on a lemma which approximates the trace of the matrix $M(k)$ given above. For q small, this theorem does not provide any particularly useful information. However, for large q the Revival Theorem proves that the probability distribution of a quantum walk will approximately return to its initial state at time $t = nq$ for $n \in \mathbb{N}$, n not significantly large. For example, if $\theta = \frac{51}{256}$, we must wait until $t \approx 10^{19}$ for revivals to cease and ballistic spread to begin.

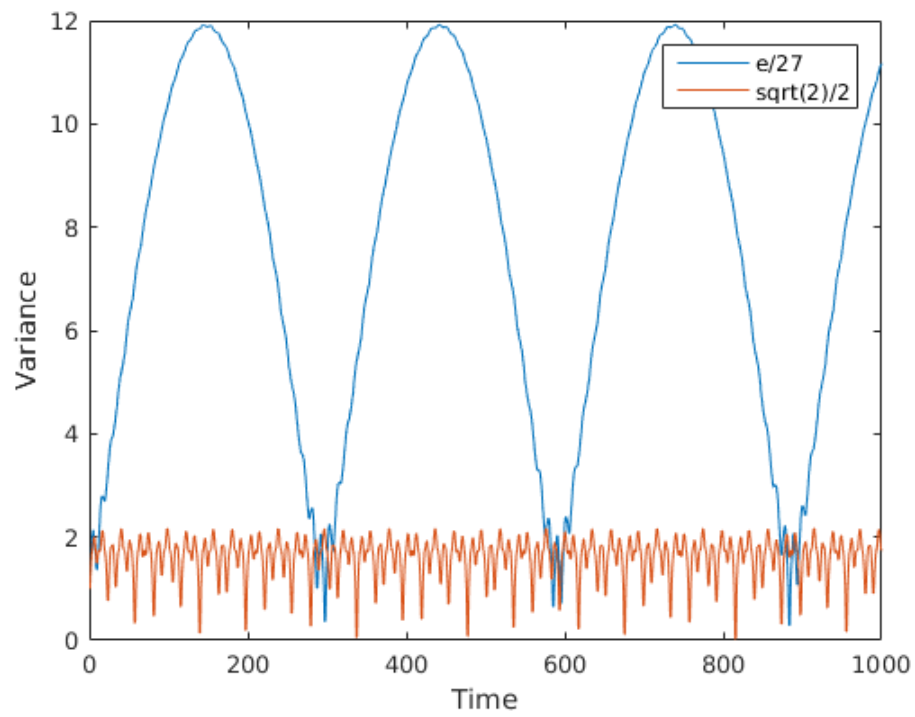


Figure 2.9: Comparison of variance over time for two irrational electric quantum walks. The walk for which $\theta = \frac{2\pi e}{27}$ exhibits returns at regularly spaced intervals while $\theta = \frac{\sqrt{2}}{2}$ leads to extremely localized behavior

Cedzich et. al. [20] also make a distinction between the “approximately rational” and “very irrational” cases of the electric quantum walk. Let x have a continued fraction representation $\{c_0, c_1, \dots\}$ and let the corresponding rational approximants be given by the sequence $\{\frac{p_0}{q_0}, \frac{p_1}{q_1}, \dots\}$. Speaking loosely, we say that x is *approximately rational* if there exists a subsequence $\{c_{n_k}\}$ of $\{c_n\}$ such that $c_{n_k} \rightarrow \infty$. If $\theta = 2\pi x$ where x is approximately rational, we find that the initial condition is increasingly well replicated at time q_{n_k} or time $2q_{n_k}$. If x is not approximately rational, as is the case with the golden ratio $x = \varphi = \frac{1+\sqrt{5}}{2}$, numerical simulations show that there are many revivals at seemingly irregular times. This behavior is known as *Anderson localization* [11] and occurs in sufficiently disordered quantum systems.

2.6 Conclusion

In this paper we have computed precise asymptotics for the general one-dimensional two-state quantum walk and illustrated regions of non-decay for a variety of two dimensional quantum walks. In addition, we have provided a brief overview of inhomogeneous quantum walks using simulations and showed that aperiodic inhomogeneities break down ballistic behavior (spread that is linear in time). In future studies, it will be worthwhile to compute precisely algebraic identities governing regions of polynomial decay for more unwieldy quantum walks such as the two dimensional tensor walk and the d -dimensional Grover walk.

Chapter 3

Absorption Probabilities of Quantum Walks

Quantum walks are known to have nontrivial interaction with absorbing boundaries. In particular, Ambainis et. al. [9] showed that in the (\mathbb{Z}, C_1, H) quantum walk (one-dimensional Hadamard walk) an absorbing boundary partially reflects information. These authors also conjectured that the left absorption probabilities $P_n^{(1)}(1, 0)$ related to the finite absorbing Hadamard walks $(\mathbb{Z}, C_1, H, \{0, n\})$ satisfy a linear fractional recurrence in n (here $P_n(1, 0)$ is the probability that a Hadamard walk particle initialized in $|1\rangle|R\rangle$ is eventually absorbed at $|0\rangle$ and not at $|n\rangle$). This result, as well as a third order linear recurrence in initial position m of $P_n^{(m)}(1, 0)$, was later proved by Bach and Borisov [12] using techniques from complex analysis. In this document we extend these results to general two state quantum walks and three-state Grover walks, while providing a partial calculation for absorption in d -dimensional Grover walks by a $d - 1$ -dimensional wall. In all of these cases, we find partial reflection of information, a linear fractional recurrence in lattice size, and a linear recurrence in initial position. In addition, we show that electric quantum walks parameterized by $\theta \in \mathbb{Q}$ have similar absorption properties as the (\mathbb{Z}, C_1, U) quantum walk while those parameterized by $\theta \notin \mathbb{Q}$ share properties with the classical random walk.

3.1 Introduction

The quantum walk is a unitary analogue of the classical random walk. Several introductory papers have been written on quantum walks which explore their use in algorithms for quantum computers and other mathematical properties [40] [65]. The quantum walk differs

from the classical random walk in many ways including its linear spreading and initial condition-dependent asymmetries. In this paper, we direct our attention to the absorption problem; that is, we wish to calculate the probability that a quantum walk particle is eventually absorbed by a collection of absorption units present in the system. By an absorption unit, we mean an element g of the group G that the walk takes place on such that if the quantum particle is observed at the location of the unit, then the particle is absorbed and the walk is terminated. Otherwise, we continue to alternate the quantum walk operator with measurements.

Solutions to the absorption problem are well known in the symmetric classical random walk [60] [46]. The one dimensional classical symmetric random walk is recurrent, meaning that a random walk particle will eventually return to its starting location (and by extension any other location on the line) with probability 1. Thus, in the semi-infinite random walk where there is a single absorbing boundary at the origin, the classical random walker particle will be absorbed there with probability 1. This property also holds for the two dimensional random walk but not for random walks of dimension three and higher [35] [16]. In addition, consider the classical finite absorbing random walk in which there are absorbing boundaries at positions 0 and N . If the particle starts at position 1, it has been shown that the probability that the particle will eventually be absorbed by the left boundary is equal to $1 - \frac{1}{N}$. Notice that as $N \rightarrow \infty$, this probability approaches 1, so in some way the finite absorption probability limits to the semi-infinite semi-infinite. These results can be generalized to asymmetric random walks, and while these walks are not recurrent, we again find that the finite absorption probabilities limit to the semi-infinite absorption probabilities.

The absorption problem for the one dimensional quantum walk is much more nuanced than the classical absorption problem. Ambainis et. al. [9] first considered the absorption problem for both the semi-infinite Hadamard walk and the finite Hadamard walk. Following their notation, let p_∞ be the probability that a Hadamard walk particle initialized in $|1\rangle|R\rangle$ is eventually absorbed at $|0\rangle$, and let p_n be the probability that the Hadamard walk particle

initialized at $|1\rangle|R\rangle$ is eventually absorbed at $|0\rangle$ if there exists another absorbing boundary at $|n\rangle$. Ambainis et. al. proved that $p_\infty = \frac{2}{\pi}$ using properties of the Catalan numbers and they also proved that $\lim_{n \rightarrow \infty} p_n = \frac{1}{\sqrt{2}}$. These two calculations directly oppose the two key properties we highlighted about the absorption problem for the classical random walk; namely, the quantum walk is not recurrent, and the finite absorption probability does not limit to the semi-infinite absorption probability. Paradoxically, these authors showed that the presence of an absorbing boundary very far away from the origin actually *increases* the probability of eventual absorption on the left.

In this same paper, Ambainis et. al. conjectured a recursion governing the finite absorption probabilities, namely $p_{n+1} = \frac{1+2p_n}{2+2p_n}$. Partial progress toward proving this result was made by Konno et. al. [44] and Bach et. al. [13] before finally being proved by Bach and Borisov [12]. This result was obtained by using the integral representation of the Hadamard product along with a few key observations from complex analysis. These authors also cited a recursion governing the absorption probabilities based on initial position. If $p_n^{(m)}$ is the probability that the Hadamard walk particle initialized at $|m\rangle|R\rangle$ is absorbed at $|0\rangle$ given an additional boundary at $|n\rangle$, then the following formula holds:

$$p_n^{(m+3)} - 7p_n^{(m+2)} + 7p_n^{(m+1)} - p_n^{(m)} = 0.$$

These results were extended to the three-state Grover walk in Wang et. al. [67] where it was discovered that those absorption probabilities satisfy $p_{n+1} = \frac{2+3p_n}{3+4p_n}$.

In this paper, we extend the described results to a more general collection of quantum walks. We find that the absorption probabilities for all of these walks share three key properties; these properties are partial reflection of information at the boundary, a linear fractional recurrence in domain size, and a linear recurrence in initial position, which is found to be independent of the initial spin state. The workflow for these calculations is consistent between examples. First, we define generating functions for which the t^{th} coefficient of the Taylor expansion corresponds to the amplitude at the absorbing unit at

time t . These generating functions can be explicitly computed using path counting arguments. From here, the absorption probability may be obtained by evaluating a Hadamard product of these generating functions at 1. The Hadamard product has an integral representation which for semi-infinite walks may be directly integrated. For the finite walks, the corresponding integrand can be separated by means of a partial fractions expansion. The partial fractions contain specific collections of poles that facilitate applications of the residue theorem.

Before proceeding to the results, we briefly discuss the electric quantum walk (EQW) [55] [20]. The EQW is a space-inhomogeneous walk on the line parameterized by $\theta \in [0, 2\pi)$. When $\theta \in 2\pi\mathbb{Q}$, the inhomogeneities are periodic and the system can be reorganized into a one dimensional quantum walk with more internal states. If however $\theta \notin 2\pi\mathbb{Q}$, these inhomogeneities are aperiodic. We will prove a result that in the semi-infinite case, the EQW is recurrent for $\theta \notin 2\pi\mathbb{Q}$ and is transient otherwise.

In Section 3.2, we discuss the definitions and methods necessary to carry out our computations. In Section 3.3, we compute absorption probabilities for the classical random walk as an initial case. The remaining sections are devoted to computing absorption probabilities for specific variants of the quantum walk. These include the general two-state one-dimensional quantum walk in Section 3.4, the three-state one-dimensional Grover walk in Section 3.5, the d -dimensional Grover walk in Section 3.6, and the two-state one-dimensional EQW in Section 3.7.

3.2 Definitions and Methods

The quantum walk has a natural generalization on groups.

Definition 3.1 *Let (G, \cdot) be a group, let $\Sigma \subset G$ where $|\Sigma| = n$, and let $U \in U(n)$ where $U(n)$ is the set of $n \times n$ unitary matrices. The quantum walk operator $Q : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ corresponding to the triple (G, Σ, U) may be written as $Q = T(I \otimes U)$ where for $g \in G$ and $\sigma \in \Sigma$, $T : |g\rangle|\sigma\rangle \mapsto |g \cdot \sigma\rangle|\sigma\rangle$. We denote this correspondence as $Q \leftrightarrow (G, \Sigma, U)$.*

The pair (G, Σ) can be thought of as an undirected Cayley graph which could admit loops [24].

We must also define an absorption unit for quantum walks. To this end, we formally define the measurement operator. Let $b \in G \times \Sigma$. The measurement operator $\Pi_{\text{yes}}^b : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ is a projection onto $|b\rangle$ while Π_{no}^b is a projection onto the subspace spanned by the states corresponding to elements in $G \setminus b$. The probabilistic interpretation of quantum mechanics dictates that if we measure a state $\psi \in \ell^2(G \times \Sigma)$ at $|b\rangle$, the resulting state becomes $\Pi_{\text{yes}}^b \psi$ with probability $\|\Pi_{\text{yes}}^b \psi\|^2$ and $\Pi_{\text{no}}^b \psi$ with probability $\|\Pi_{\text{no}}^b \psi\|^2$. If $B \subset G \times \Sigma$, let Π_{no}^B be the composition of *no* measurement projections for all $b \in B$. In this way, we can define the quantum walk operator for an absorbing quantum walk.

Definition 3.2 *Let $Q \leftrightarrow (G, \Sigma, U)$ be a quantum walk operator and let $B \subset G \times \Sigma$. Then we say that $\Pi_{\text{no}}^B Q$ is the absorbing quantum walk operator corresponding to the ordered quadruple (G, Σ, U, B) and we denote this correspondence as $\Pi_{\text{no}}^B Q \leftrightarrow (G, \Sigma, U, B)$.*

We use the *no* operator in our definition because if we observe the particle somewhere in B , then the experiment is terminated, while if the particle is not observed in B (i.e. we are in the range of Π_{no}^B) the experiment continues.

For an absorption problem, we wish to compute the probability P that the quantum walk particle is eventually absorbed by some subset of the absorbing units $B_0 \subset B$ of an absorbing quantum walk with operator $\Pi_{\text{no}}^B Q \leftrightarrow (G, \Sigma, U, B)$ before it is absorbed anywhere else in B (i.e. before it is absorbed in $B \sim B_0$). Let $\psi \in \ell^2(G \times \Sigma)$ be the initial state. Then we can express this probability as an infinite sum:

$$P = \sum_{t=1}^{\infty} \left[\sum_{b \in B_0} |\langle b | Q (\Pi_{\text{no}}^B Q)^{t-1} | \psi \rangle|^2 \right]. \quad (3.1)$$

This paper is devoted to computing such sums for a selection of quantum walks.

Path Counting and Generating Functions

The quantum walk is a quantum Markov chain [34] and thus has a pathwise representation. We must first define a path and its associated amplitude and displacement.

Definition 3.3 Consider the quantum walk operator $Q \leftrightarrow (G, \Sigma, U)$ where $U(\sigma_1, \sigma_2)$ is the transition amplitude from internal state σ_1 to σ_2 . An n -path $\gamma \in \Sigma^{n+1}$ is represented as $\gamma = (\sigma_0, \dots, \sigma_n)$ and its associated displacement is defined as $S(\gamma) = \sum_{k=1}^n \sigma_k$. Its associated amplitude is defined as $A(\gamma) = \prod_{k=1}^n U(\sigma_{k-1}, \sigma_k)$.

In this definition, the used summation in the definition of $S(\gamma)$ indicates that here the binary group operations defined notationally as sums rather than products. This is done to be consistent with most applications of these particular results. Let $\varphi_k : \Sigma^{n+1} \rightarrow \Sigma$ be the k^{th} entry of a n -path where $0 \leq k \leq n$. In view of the quantum walk as a quantum Markov chain, the following pathwise representation holds [34]

Proposition 3.1 Consider the quantum walk operator $Q \leftrightarrow (G, \Sigma, U)$ and let us define a set of paths where $g_0, g_1 \in G$ and $\sigma_0, \sigma_1 \in \Sigma$:

$$\Gamma = \{\gamma \in \Sigma^{n+1} : \varphi_0(\gamma) = \sigma_0, \varphi_n(\gamma) = \sigma_1, S(\gamma) = g_0 \cdot g_1^{-1}\}. \quad (3.2)$$

Then:

$$\langle g_1, \sigma_1 | Q^n | g_0, \sigma_0 \rangle = \sum_{\gamma \in \Gamma} A(\gamma). \quad (3.3)$$

This is closely related to the path integral formulation of quantum mechanics proposed by Feynman [30].

With a little care, a pathwise representation of amplitudes for absorbing quantum walks can also be written. To this end let $\theta_k : \Sigma^{n+1} \rightarrow \Sigma^{k+1}$ be the restriction of an n -path $\gamma = (\sigma_0, \dots, \sigma_n)$ to a k -path $\theta_k(\gamma) = (\sigma_0, \dots, \sigma_k)$ for $k \leq n$.

Proposition 3.2 *Consider the absorbing quantum walk operator $\Pi_{no}^B Q \leftrightarrow (G, \Sigma, U, B)$. If we let Γ be the set from the previous proposition, then we define a new set of paths:*

$$\Gamma' = \Gamma \cap \{\gamma \in \Sigma^{n+1} : S(\theta_k(\gamma)) \cdot g_0 \notin B \ \forall k \leq n\}. \quad (3.4)$$

Then the following holds:

$$\langle g_1, \sigma_1 | (\Pi_{no}^B Q)^n | g_0, \sigma_0 \rangle = \sum_{\gamma \in \Gamma'} A(\gamma). \quad (3.5)$$

The proof of this proposition follows easily from proposition 2.1.

In view of the absorbing probability equation above, we consider for a complex variable z generating functions $f_{b|\psi}(z)$ for an absorbing quantum walk defined as:

$$f_{b|\psi}(z) = \sum_{t=1}^{\infty} \langle b | Q (\Pi_{no}^B Q)^{t-1} | \psi \rangle z^t. \quad (3.6)$$

We use the propositions above to consider a pathwise representation of these generating functions:

Definition 3.4 *Let $f_{b|\psi}(z)$ be a generating function for an absorbing quantum walk (G, Σ, U, B) where $\psi = (g_0, \sigma_0)$ and $b = (g_1, \sigma_1)$. We define the set $F_{b|\psi}^{(n)}$ of associated n -paths of this generating function as:*

$$F_{b|\psi}^{(n)} = \{\gamma \in \Sigma^{n+1} : \varphi_0(\gamma) = \sigma_0, \varphi_n(\gamma) = \sigma_1, S(\gamma) = g_0 \cdot g_1^{-1}, S(\theta_k(\gamma)) \cdot g_0 \notin B \ \forall k < n\} \quad (3.7)$$

By using a substitution from Proposition 3.2, the generating functions may be rewritten as:

$$f_{b|\psi}(z) = \sum_{t=1}^{\infty} \left(\sum_{\gamma \in F_{b|\psi}^{(t)}} A(\gamma) \right) z^t. \quad (3.8)$$

Now that we have a pathwise representation of the generating functions, we will be able to write self-referential relations then dividing up associated paths in certain ways. We consider one of these:

Proposition 3.3 *Let $\Pi_{no}^B Q \leftrightarrow (G, \Sigma, U, B)$ be an absorbing quantum walk operator and let $f_{b|\psi}(z)$ be a generating function. If $\psi = (g_0, \sigma_0) \equiv |g_0\rangle|\sigma_0\rangle$, let $\Sigma' = \{\sigma \in \Sigma : g_0 \cdot \sigma \notin B\}$. Then:*

$$f_{b|\psi}(z) = \langle b|Q|\psi\rangle z + z \sum_{\sigma \in \Sigma'} f_{b|(g_0 \cdot \sigma)}(z). \quad (3.9)$$

We call equation (3.9) in this proposition a *first step transformation*. The proof of the proposition is simple and easily seen from separating the first term from the generating function in the Taylor expansion. The generating functions in the summation on the right will typically be related to the generating function on the left in some way after considering a second transformation. This second transformation we consider is more involved. To this end consider the definition:

Definition 3.5 *Let $\Pi_{no}^B Q \leftrightarrow (G, \Sigma, U, B)$ be an absorbing quantum walk operator and let $\psi = (g_0, \sigma_0) \equiv |g_0\rangle|\sigma_0\rangle$. If there exists a set $X \subset G \times \Sigma$ such that, for every $n \in \mathbb{N}$ and $\gamma \in F_{b|\sigma}^{(n)}$, there exists a $k < n$ such that $(S(\text{theta}_j(\gamma)), \varphi_j(\gamma)) \notin X$ for $j < k$ and $(S(\text{theta}_k(\gamma)), \varphi_k(\gamma)) \in X$, then we say the generating function $f_{b|\psi}(z)$ is segmented by X .*

The generating functions for one dimensional quantum walks are typically segmented by a single element, but in higher dimensions the segmenting sets are larger. We now prove the *segmenting transformation* in the following proposition:

Proposition 3.4 *Let $\Pi_{no}^B Q \leftrightarrow (G, \Sigma, U, B)$ be an absorbing quantum walk operator and let $f_{b|\psi}(z)$ be a generating function segmented by X . Then we have:*

$$f_{b|\psi}(z) = \sum_{\psi' \in X} f_{b|\psi'}(z) f_{\psi'|\psi}(z) \quad (3.10)$$

Proof: Since $f_{b|\psi}(z)$ is segmented by X , for every $\gamma \in F_{b|\psi}^{(n)}$ there exists a $k < n$ and an element $\psi' \in X$ such that $theta_k(\gamma) \in F_{\psi'|\psi}^{(k)}$, and if $theta'_k : \Sigma^{n+1} \rightarrow \Sigma^{k+1}$ restricts an n -path $\gamma = (\sigma_0, \dots, \sigma_n)$ to the k -path $theta'_k(\gamma) = (\sigma_k, \dots, \sigma_n)$, then $theta'_{n-k}(\gamma) \in F_{b|\psi'}^{(n-k)}$. This implies:

$$\sum_{\gamma \in F_{b|\psi}^{(n)}} A(\gamma) = \sum_{\psi' \in X} \left[\sum_{k=1}^n \left(\sum_{\gamma_1 \in F_{\psi'|\psi}^{(k)}} A(\gamma_1) \right) \left(\sum_{\gamma_2 \in F_{b|\psi'}^{(n-k)}} A(\gamma_2) \right) \right].$$

The result follows from recognizing the formula of the product of two Taylor series. \square

Using these two transformations in tandem allow us to write a self-referential relation among generating functions, upon which we can derive closed forms. For the semi-infinite walks, these closed forms may be computed explicitly. However, in finite cases the generating functions satisfy recursions in the size of the lattice. We solve the closed forms of functions $f_n(z)$ satisfying

$$f_{n+1}(z) = \frac{af_n(z) + b}{cf_n(z) + d} \quad (3.11)$$

where $f_1(z) = 0$. We compute a closed form expression of $f_n(z)$ in the following lemma:

Lemma 3.1 *Let $\{f_n(z)\}$ be a sequence of functions satisfying (13) and let $f_1(z) = 0$. If we let $\lambda_{\pm}(z) = \frac{1}{2} \left[a + d \pm \sqrt{(a+d)^2 - 4(ad-bc)} \right]$ and $F_n(z) = \lambda_+(z)^n - \lambda_-(z)^n$, then:*

$$f_n(z) = \frac{bF_{n-1}(z)}{F_n(z) - aF_{n-1}(z)} \quad (3.12)$$

The proof of this lemma follows from considering this recursion as a matrix multiplication. The coefficients $\{a, b, c, d\}$ will typically be polynomials in z . We will also find the following recurrence governing $F_n(z)$ useful:

$$F_{n+2}(z) - (a+d)F_{n+1}(z) + (ad-bc)F_n(z) = 0 \quad (3.13)$$

Hadamard Product

In order to compute an absorption probability from the constructed generating function, we must use a construction from complex analysis called the *Hadamard product*.

Definition 3.6 Let $f(z) = \sum_{k=0}^{\infty} a_k z^k$ and $g(z) = \sum_{k=1}^{\infty} b_k z^k$. Then the Hadamard product of f and g evaluated at z is defined as follows:

$$(f \odot g)(z) = \sum_{k=0}^{\infty} a_k b_k z^k \quad (3.14)$$

This Hadamard product has an integral representation which we will use extensively:

Proposition 3.5 If γ is a contour in the w plane inside which $f(w)$ and $g\left(\frac{z}{w}\right)$ are analytic, then we may write the following:

$$(f \odot g)(z) = \frac{1}{2\pi i} \int_{\gamma} \frac{1}{w} f(w) g\left(\frac{z}{w}\right) dw \quad (3.15)$$

Proof: See [63]. □

Using this Hadamard product, one can express the absorption probability P in terms of the generating functions. Interchanging the order of summation in equation (3.1) defining P , we may write:

$$P = \sum_{b \in B_0} \left(f_{b|\psi}(z) \odot \overline{f_{b|\psi}(\bar{z})} \right) (1) \quad (3.16)$$

In general, the Hadamard product is difficult to compute, but our generating functions are in a form that makes this possible. In particular, the integrand in equation (3.15) of Proposition 3.5 can be divided via a partial fractions expansion. One of these fractions has all but a few poles contained outside the contour of integration, leading to an easy evaluation via residue theorem [6]. The other fraction has all of its poles contained inside the contour. The special form of this fraction allows us to use the following lemma:

Lemma 3.2 *Let $f : \mathbb{C} \rightarrow \mathbb{C}$ be a rational function whose poles lie in a contour γ . Further, if we write $f(z) = \frac{p(z)}{q(z)}$, let $\deg(q) > \deg(p) + 1$. Then we have:*

$$\int_{\gamma} f(z) dz = 0 \tag{3.17}$$

Proof: See [6].

3.3 One Dimensional Classical Random Walk

Before addressing absorption probabilities in the quantum walk, we compute absorption probabilities of the one dimensional classical random walk to illustrate what we mean by “classical behavior”. While we opt to use language from probability theory in this section, the path counting arguments from the previous section will carry over. We need not compute any Hadamard products since the random walk is a Markov chain and not a quantum Markov chain.

We must first formally define the classical random walk:

Definition 3.7 *A classical random walk is a sequence of random variables $\{X_j\}_{j=0}^{\infty}$ which satisfy $P(X_{t+1} = X_t + 1) = p$ and $P(X_{t+1} = X_t - 1) = q = 1 - p$.*

Notice that the quantum n -paths we previously defined are transition-based. To carry over our path counting methods, we must reassess this definition:

Definition 3.8 *An n -path is an element $\gamma \in \{-1, 1\}^n$ written as $\gamma = (x_1, \dots, x_n)$. We say that the associated displacement of γ is $S(\gamma) = \sum_{k=1}^n x_k$ while the associated probability of γ is $P(\gamma) = p^{(n+S(\gamma))/2} q^{(n-S(\gamma))/2}$.*

Semi-Infinite Case

Let us consider a classical random walk for which $X_0 = m > 0$ and let there be an absorbing boundary at position 0. We want to calculate the absorption probability $P_{\infty}^{(m)}$ that the

particle is eventually absorbed at position 0. The absorption probability may be written as:

$$P_\infty^{(m)} = \sum_{t=1}^{\infty} P(X_t = 0 | X_0 = m, X_j > 0 \forall j < t).$$

This probability has a convenient pathwise representation. If we let $\Gamma_n = \{\gamma \in \{-1, 1\}^n : S(\gamma) = -m, S(\text{theta}_k(\gamma)) > -m \forall k < n\}$, then we can write the following:

$$P_\infty^{(m)} = \sum_{t=1}^{\infty} \left(\sum_{\gamma \in \Gamma_t} P(\gamma) \right).$$

From this equation we construct a collection of generating functions:

$$f_\infty^{(m)}(z) = \sum_{t=1}^{\infty} \left(\sum_{\gamma \in \Gamma_t} P(\gamma) \right) z^t.$$

It is clear that $P_\infty^{(m)} = f_\infty^{(m)}(1)$. It remains to compute a closed form for $f_\infty^{(m)}(z)$. Since $f_\infty^{(m)}(z)$ is segmented by $m - 1$, we can use a segmenting transformation and induction to find:

$$f_\infty^{(m)}(z) = f_\infty^{(1)}(z) f_\infty^{(m-1)}(z) = \left(f_\infty^{(1)}(z) \right)^m.$$

We have reduced this absorption problem to understanding the function $f(z) = f_\infty^{(1)}(z)$. By a first step transformation and substituting the previous relation, we find:

$$f(z) = qz + pz f(z)^2.$$

The function $f(z)$ satisfies a quadratic equation, but there is a bit of subtlety in selecting the proper solution. To keep $f(0)$ well defined, we choose the following solution:

$$f(z) = \begin{cases} \frac{1}{2p} \left[1 - \sqrt{1 - 4pqz^2} \right] & p \leq q \\ \frac{1}{2p} \left[1 + \sqrt{1 - 4pqz^2} \right] & p > q \end{cases}.$$

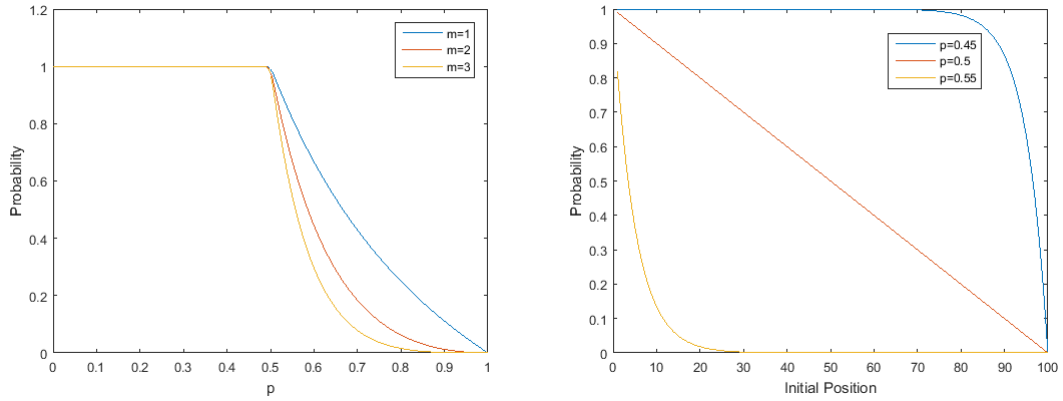


Figure 3.1: Left absorption probabilities for a random walk on a one dimensional lattice of size 100

Using this closed form we are immediately granted a solution to the absorption problem:

Theorem 3.1 *The absorption probabilities $P_\infty^{(m)}$ satisfy:*

$$P_\infty^{(m)} = \begin{cases} 1 & p \leq q \\ \left(\frac{q}{p}\right)^m & p > q \end{cases}. \quad (3.18)$$

Finite Case

The finite case is solved in much the same way as the semi-infinite case was. Let us consider a random walk for which $X_0 = m$ and there are two absorbing boundaries, one at position 0 and another at position n . We wish to find the absorption probability $P_n^{(m)}$ that the particle is eventually absorbed at position 0 and not at n . We write this as:

$$P_n^{(m)} = \sum_{t=1}^{\infty} P(X_t = 0 | X_0 = m, 0 < X_j < n \quad \forall j < t).$$

This probability also has a pathwise representation. Considering Γ_n from the previous section, define $\Gamma'_t = \Gamma_t \cap \{\gamma \in \{-1, 1\}^t : S(\theta_{a_k}(\gamma)) < n - m \quad \forall k \leq t\}$. Then we can write

the following:

$$P_n^{(m)} = \sum_{t=1}^{\infty} \left(\sum_{\gamma \in \Gamma'_t} P(\gamma) \right).$$

We construct the obvious class of generating functions from these absorption probabilities:

$$f_n^{(m)}(z) = \sum_{t=1}^{\infty} \left(\sum_{\gamma \in \Gamma'_t} P(\gamma) \right) z^t.$$

Here, it is clear that $P_n^{(m)} = f_n^{(m)}(1)$, so it remains to gather closed forms of these generating functions. The segmenting transformation is slightly different from last time; the generating function $f_n^{(m)}(z)$ is segmented by $m - 1$; however via induction we have:

$$f_n^{(m)}(z) = f_{n-m+1}^{(1)}(z) f_n^{(m-1)}(z) = \prod_{k=1}^m f_{n-m+k}^{(1)}(z).$$

It thus remains to find a closed form for the generating functions for which $m = 1$. By using a first step transformation and a subsequent substitution of the segmenting relation, we have:

$$f_n^{(1)}(z) = qz + pz f_n^{(1)}(z) f_{n-1}^{(1)}(z).$$

Thus we arrive at a linear fractional recurrence in n governing these functions:

$$f_{n+1}^{(1)}(z) = \frac{qz}{1 - pz f_n^{(1)}(z)}.$$

Here, $f_1^{(1)}(z) = 0$. Using results from Lemma 2.1, we arrive at a closed form for $f_n^{(1)}(z)$:

$$f_n^{(1)}(z) = qz \frac{F_{n-1}(z)}{F_n(z)}.$$

Here, $F_n(z) = \lambda_+(z)^n - \lambda_-(z)^n$ and $\lambda_{\pm}(z) = \frac{1}{2} \left[1 \pm \sqrt{1 - 4pqz^2} \right]$. Recognize that $\lambda_+(1) = q$ and $\lambda_-(1) = p$. If $p \neq q$, then we have $P_n^{(1)} = q \left(\frac{p^{n-1} - q^{n-1}}{p^n - q^n} \right)$, but if $p = q$, we find $P_n^{(1)} = 1 - \frac{1}{n}$. Since $P_n^{(m)} = \prod_{k=1}^m P_{n-m+k}$, a telescoping relation gives us the following:

Theorem 3.2 *The absorption probabilities $P_n^{(m)}$ satisfy the following:*

$$P_n = \begin{cases} q^m \left(\frac{p^{n-m} - q^{n-m}}{p^n - q^n} \right) & p \neq q \\ 1 - \frac{m}{n} & p = q \end{cases} \quad (3.19)$$

Discussion

Before continuing to the computations involving the quantum walk, we make note of a few key characteristics these absorption probabilities share. First, notice that $P_\infty^{(m)} = 1$ if $q \leq p$. If we keep the absorbing boundary at the origin and let m be negative, a simple rearrangement of the previous results shows that $P_\infty^{(-m)} = 1$ for $p \leq q$. Combining these results, we note that the symmetric random walk for $p = q$ is recurrent; that is, the random walk will eventually visit any point on \mathbb{Z} with probability 1. As mentioned in the introduction, this holds for the classical random walk on \mathbb{Z}^2 but not on spaces of dimension 3 or higher.

Second, these absorption probabilities interchange with the limit nicely:

Theorem 3.3 *For absorption probabilities of the random walk, the following relation holds:*

$$\lim_{n \rightarrow \infty} P_n^{(m)} = P_\infty^{(m)}. \quad (3.20)$$

While this may seem like an obvious property, it will not be satisfied for the quantum walks we discuss later. We have another result if we take the limit in a different way:

Theorem 3.4 *If $0 < c < 1$, then we have:*

$$\lim_{n \rightarrow \infty} P_n^{(cn)} = \begin{cases} 0 & p > q \\ 1 - c & p = q \\ 1 & p < q \end{cases}. \quad (3.21)$$

We include this theorem because these absorption probabilities are stable in the limit taken

on a ray cn . In particular, there is a dichotomy between the cases guaranteed absorption to the left ($p < q$) and guaranteed absorption to the right ($p > q$) where the choice of ray has no impact on the probability, and the symmetric case in which the choice of ray actually does affect the absorption probability.

Lastly, we write a few recurrence relations among the absorption probabilities. The proof of these relationships is straightforward:

Theorem 3.5 *Let $P_n^{(m)}$ be an absorption probability of the random walk. Then the following formulas hold:*

$$P_{n+1}^{(1)} = \frac{q}{1 - pP_n^{(1)}}; \quad (3.22)$$

$$P_n^{(m)} = \prod_{k=1}^m P_{n-m+k}^{(1)}; \quad (3.23)$$

$$P_n^{(m+2)} - \frac{1}{p}P_n^{(m+1)} + \frac{q}{p}P_n^{(m)} = 0. \quad (3.24)$$

Proof: The first two formulas hold by letting $z = 1$ in two of the generating function relations above. The second may be derived by noting that $F_{n+2} - F_{n+1} + pqF_n = 0$ and multiplying this relation by q^{m+1} . \square

3.4 (\mathbb{Z}, C_1, U) Quantum Walk

We now compute absorption probabilities for the (\mathbb{Z}, C_1, U) quantum walk where $C_1 = \{-1, 1\}$ and U is an arbitrary 2×2 unitary matrix. It suffices to consider matrices of the form $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$, as phase constants will not affect the absorption probabilities. As

mentioned previously, the case of $U = H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ where H is the 2×2 Hadamard matrix has been studied in a few papers [9] [13] [12].

Semi-Infinite Case

We first calculate the absorption probabilities $P_\infty^{(m)}(\alpha, \beta)$ corresponding to an initial condition $|m\rangle(\alpha|R\rangle + \beta|L\rangle)$ and the quantum walk operator $\Pi_{\text{no}}^0 Q \leftrightarrow (\mathbb{Z}, C_1, U, \{0\})$. If we place an absorbing boundary at $|0\rangle$, we need only consider absorption at $|0\rangle|L\rangle$ as there will never be amplitude at $|0\rangle|R\rangle$ in this setting. We can write out the general absorption probabilities as follows:

$$P_\infty^{(m)}(\alpha, \beta) = \sum_{t=1}^{\infty} |\alpha|^2 |\langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, R\rangle|^2 + \sum_{t=1}^{\infty} |\beta|^2 |\langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, L\rangle|^2 + \sum_{t=1}^{\infty} 2\text{Re} \left[\alpha\bar{\beta} \langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, R\rangle \overline{\langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, L\rangle} \right]. \quad (3.25)$$

Recognize the first two quantities in this sum as $|\alpha|^2 P_\infty^{(m)}(1, 0) + |\beta|^2 P_\infty^{(m)}(0, 1)$. If we define $H_\infty^{(m)} = \sum_{t=1}^{\infty} \langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, R\rangle \overline{\langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, L\rangle}$, then we may rewrite the general absorption probability as:

$$P_\infty^{(m)}(\alpha, \beta) = |\alpha|^2 P_\infty^{(m)}(1, 0) + |\beta|^2 P_\infty^{(m)}(0, 1) + 2\text{Re} \left[\alpha\bar{\beta} H_\infty^{(m)} \right]. \quad (3.26)$$

We illustrate the calculation of $P_\infty^{(1)}(1, 0)$. A simple observation can extend this to $P_\infty^{(1)}(\alpha, \beta)$.

Generating Functions

We first define the following two generating functions:

$$r_\infty^{(m)}(z) = \sum_{t=1}^{\infty} \langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, R\rangle z^t, \quad l_\infty^{(m)}(z) = \sum_{t=1}^{\infty} \langle 0, L|Q(\Pi_{\text{no}}^0 Q)^{t-1}|m, L\rangle z^t.$$

We use this subsection to prove the following proposition:

Proposition 3.6 *The generating functions $r_\infty^{(m)}(z)$ and $l_\infty^{(m)}(z)$ have the following closed forms:*

$$r_\infty^{(m)}(z) = \frac{a}{b} \left(\frac{1}{2az} \right)^m \left(1 - z^2 - \sqrt{z^4 + 2(|b|^2 - |a|^2)z^2 + 1} \right) \quad (3.27)$$

$$\times \left(1 + z^2 - \sqrt{z^4 + 2(|b|^2 - |a|^2)z^2 + 1} \right)^{m-1} \quad (3.28)$$

$$l_\infty^{(m)}(z) = \left(\frac{1}{2az} \right)^m \left(1 + z^2 - \sqrt{z^4 + 2(|b|^2 - |a|^2)z^2 + 1} \right)^m \quad (3.29)$$

Proof: Both of these generating functions are segmented by $|m-1\rangle|L\rangle$. Using a segmenting transformation and induction, the following relationships hold:

$$r_\infty^{(m)}(z) = r_\infty^{(1)}(z) \left(l_\infty^{(1)}(z) \right)^{m-1}, \quad l_\infty^{(m)}(z) = \left(l_\infty^{(1)}(z) \right)^m.$$

It now remains to handle the $m = 1$ generating functions. Using a first step transformation and substituting this segmenting relation, we arrive at the system:

$$r_\infty^{(1)}(z) = -\bar{b}z + azr_\infty^{(1)}(z)l_\infty^{(1)}(z), \quad l_\infty^{(1)}(z) = \bar{a}z + bZR_\infty^{(1)}(z)l_\infty^{(1)}(z).$$

This system can be solved simply and results in the following solutions:

$$r_\infty^{(1)}(z) = \frac{1}{2bz} \left[1 - z^2 - \sqrt{z^4 + 2(|b|^2 - |a|^2)z^2 + 1} \right].$$

$$l_\infty^{(1)}(z) = \frac{1}{2az} \left[1 + z^2 - \sqrt{z^4 + 2(|b|^2 - |a|^2)z^2 + 1} \right]. \quad (3.30)$$

We choose the negative square root so that these generating functions have a convergent Taylor series about $z = 0$. The main result follows upon substitution. \square

Hadamard Product

The absorption probabilities may be written in terms of the generating functions as follows:

$$P_\infty^{(m)}(1, 0) = \left(r_\infty^{(m)}(z) \odot \overline{r_\infty^{(m)}(\bar{z})} \right) (1), \quad P_\infty^{(m)}(0, 1) = \left(l_\infty^{(m)}(z) \odot \overline{l_\infty^{(m)}(\bar{z})} \right) (1).$$

$$H_\infty^{(m)} = \left(r_\infty^{(m)}(z) \odot \overline{l_\infty^{(m)}(\bar{z})} \right) (1). \quad (3.31)$$

Presently, we are only able to state the semi-infinite absorption probabilities for the $m = 1$ case. For the $U = H$ case, Ambainis et. al. used an appeal to the Catalan numbers to prove that $P_\infty^{(1)}(1, 0) = \frac{2}{\pi}$. However, this approach does not generalize well to the general unitary matrix case and we opt to use the integral expression of the Hadamard product outright in our proof.

Theorem 3.6 *The following formula holds:*

$$P_\infty^{(1)}(1, 0) = \frac{1}{2|b|^2} \left[|b|^2 - |a|^2 + \frac{4|a||b|}{\pi} + \frac{2}{\pi} (|b|^2 - |a|^2) \sin^{-1}(|b|^2 - |a|^2) \right] \quad (3.32)$$

Here, $\sin^{-1} : [-1, 1] \rightarrow [-\frac{\pi}{2}, \frac{\pi}{2}]$. If we write $|a| = \sin \phi$ where $\phi \in [0, \frac{\pi}{2}]$, then we also have:

$$P_\infty^{(1)}(1, 0) = \frac{\sin 2\phi + (\pi - 2\phi) \cos 2\phi}{\pi \cos^2 \phi} \quad (3.33)$$

Proof: From Ambainis et. al. we are able to alter the integral representation of the Hadamard product slightly:

$$P_\infty^{(1)} = \frac{1}{2\pi} \int_0^{2\pi} |r_\infty^{(1)}(e^{i\theta})|^2 d\theta.$$

This may be integrated outright. □

The general absorption probability $P_\infty^{(1)}(\alpha, \beta)$ will be handled in the discussion at the end of the section.

Finite Case

Let $\Pi_{\text{no}}^n \Pi_{\text{no}}^0 Q \leftrightarrow (\mathbb{Z}, C_1, U, \{0, n\})$ be an absorbing quantum walk operator corresponding to the quantum walk on the finite one dimensional lattice. We are interested in the absorption probabilities $P_n^{(m)}(\alpha, \beta)$ or the probability that a quantum walk particle initialized in $|m\rangle(\alpha|R\rangle + \beta|L\rangle)$ is eventually absorbed at $|0\rangle$ in the presence of another absorbing boundary at $|n\rangle$. We can divide the general absorption probability as we had in the previous section:

$$P_n^{(m)}(\alpha, \beta) = |\alpha|^2 P_n^{(m)}(1, 0) + |\beta|^2 P_n^{(m)}(0, 1) + 2\text{Re} \left[\alpha \bar{\beta} H_n^{(m)} \right]. \quad (3.34)$$

Again, we will be focusing most of our attention on computing $P_n^{(m)}(1, 0)$, as the other two quantities are calculated similarly.

Generating Functions

Let us define the generating functions:

$$r_n^{(m)}(z) = \sum_{t=1}^{\infty} \langle 0, L | Q(\Pi_{\text{no}}^n \Pi_{\text{no}}^0 Q)^{t-1} | m, R \rangle z^t, \quad l_n^{(m)}(z) = \sum_{t=1}^{\infty} \langle 0, L | Q(\Pi_{\text{no}}^n \Pi_{\text{no}}^0 Q)^{t-1} | m, L \rangle z^t.$$

This section is devoted to computing the following closed form of these generating functions:

Proposition 3.7 *We have:*

$$r_n^{(m)}(z) = \frac{-\bar{b}\bar{a}^{m-1}z^m R_{n-m}(z)}{R_n(z) - z^2 R_{n-1}(z)}, \quad l_n^{(m)}(z) = \bar{a}^m z^m \left(\frac{R_{n-m}(z) - z^2 R_{n-m-1}(z)}{R_n(z) - z^2 R_{n-1}(z)} \right). \quad (3.35)$$

Proof: Both of these generating functions are segmented by $|m-1\rangle|L\rangle$. Using a combination of the segmenting transformation and induction, we may write the generating

functions using $m = 1$ generating functions:

$$r_n^{(m)}(z) = r_{n-m+1}^{(1)}(z) \prod_{k=2}^m l_{n-m+k}^{(1)}(z), \quad l_n^{(m)}(z) = \prod_{k=1}^m l_{n-m+k}^{(1)}(z).$$

Using a first step transformation along with this formula, we arrive at the following system:

$$r_n^{(1)}(z) = -\bar{b}z + azr_{n-1}^{(1)}(z)l_n^{(1)}(z), \quad l_n^{(1)}(z) = \bar{a}z + bZR_{n-1}^{(1)}(z)l_n^{(1)}(z).$$

These two formulas can be combined to construct a recursion for $r_n^{(1)}(z)$:

$$r_{n+1}^{(1)}(z) = \frac{z^2 r_n^{(1)}(z) - \bar{b}z}{bZr_n^{(1)}(z) - 1}.$$

By using lemma 3.1, we can solve for the following closed form:

$$r_n^{(1)}(z) = \frac{-\bar{b}zR_{n-1}(z)}{R_n(z) - z^2R_{n-1}(z)}.$$

Here, $R_n(z) = \lambda_+(z)^n - \lambda_-(z)^n$ and $\lambda_{\pm}(z) = \frac{1}{2} \left[(1 + z^2) \pm \sqrt{z^4 + 2(|b|^2 - |a|^2)z^2 + 1} \right]$.
 Meanwhile, by recognizing $l_n^{(1)}(z) = \frac{b}{a}r_n^{(1)}(z) + \frac{z}{a}$ and using the recursion relation $R_{n+1}(z) - z^2R_n(z) = R_n(z) - |a|^2z^2R_{n-1}(z)$, we can calculate:

$$l_n^{(1)}(z) = \bar{a}z \left(\frac{R_{n-1}(z) - z^2R_{n-2}(z)}{R_n(z) - z^2R_{n-1}(z)} \right).$$

Applying induction and the segmenting relation derives the result. □

Hadamard Product

We will detail the computation of $P_n^{(m)}(1, 0) = \left(r_n^{(m)}(z) \odot \overline{r_n^{(m)}(\bar{z})} \right) (1)$ while noting that $P_n^{(m)}(0, 1) = \left(l_n^{(m)}(z) \odot \overline{l_n^{(m)}(\bar{z})} \right) (1)$ and $H_n^{(m)} = \left(r_n^{(m)}(z) \odot \overline{l_n^{(m)}(\bar{z})} \right) (1)$. We wish to use the integral representation of these Hadamard products as given by proposition 3.5, so we must provide a region for which the generating functions are analytic. En route to this we

require a lemma:

Lemma 3.3 *Let $f(w, z) = \frac{z^2 w - \bar{b}z}{-bz w + 1}$ where $|b| < 1$. Then $|w|, |z| \leq 1 \Rightarrow |f(w, z)| \leq 1$.*

Proof: Let us rewrite $f(w, z)$ as:

$$f(w, z) = \frac{w - \frac{\bar{b}}{z}}{-bz w + 1}.$$

First consider the function $g_z(w) = f(w, z)$ where z is fixed. If $|z| = 1$, then it follows that $g_z(w)$ is an automorphism of the unit disk. Next consider the function $h_w(z) = f(w, z)$ where w is fixed. For $|w| \leq 1$, $h_w(z)$ is analytic in the unit disk since there is a single pole located at $z = \frac{1}{bw}$. The result now follows from the maximum modulus principle. \square

This lemma allows us to prove the following proposition:

Proposition 3.8 *For every $m, n \in \mathbb{N}$, there exists an $\epsilon > 0$ such that $r_n^{(m)}(z)$ and $l_n^{(m)}(z)$ are analytic in the disk $|z| < 1 + \epsilon$.*

Proof: Via induction, the previous lemma shows that $|z| \leq 1 \Rightarrow |r_n^{(1)}(z)| \leq 1$ for all $n \in \mathbb{N}$, and a continuity argument tells us that for every $n \in \mathbb{N}$ there exists an $\epsilon > 0$ such that $r_n^{(1)}(z)$ is analytic in the disk $|z| < 1 + \epsilon$. Since $l_n^{(1)}(z) = \frac{b}{a} r_n^{(1)}(z) + \frac{z}{a}$, this conclusion must also hold for $l_n^{(1)}(z)$. Since $r_n^{(m)}(z)$ and $l_n^{(m)}(z)$ are products of these $m = 1$ generating functions, the result follows. \square

Before moving onto the computation of the Hadamard product, we prove two lemmas which will aid in this endeavor:

Lemma 3.4 *The following formulas hold:*

$$\overline{r_n^{(m)}\left(\frac{1}{\bar{z}}\right)} = \frac{-ba^{m-1}z^m R_{n-m}(z)}{R_n(z) - R_{n-1}(z)}, \quad \overline{l_n^{(m)}\left(\frac{1}{\bar{z}}\right)} = a^m z^m \frac{R_{n-m}(z) - R_{n-m-1}(z)}{R_n(z) - R_{n-1}(z)} \quad (3.36)$$

Proof: The result follows from noting that $\overline{\lambda_{\pm}\left(\frac{1}{\bar{z}}\right)} = \frac{1}{z^2} \lambda_{\mp}(z)$ and $\overline{R_n\left(\frac{1}{\bar{z}}\right)} = \left(\frac{1}{z^2}\right)^n R_n(z)$.

\square

Lemma 3.5 *The following formula holds:*

$$\begin{aligned} & \frac{R_{n-m}(z)}{(R_n(z) - z^2 R_{n-1}(z))(R_n(z) - R_{n-1}(z))} \\ &= \frac{1}{|a|^{2m-2} z^{2m-2} (1-z^2) R_1(z)} \left[\frac{R_m(z) - R_{m-1}(z)}{R_n(z) - R_{n-1}(z)} - \frac{R_m(z) - z^2 R_{m-1}(z)}{R_n(z) - z^2 R_{n-1}(z)} \right]. \end{aligned} \quad (3.37)$$

Proof: Let us assume the following relation holds:

$$\frac{R_{n-m}(z)}{(R_n(z) - z^2 R_{n-1}(z))(R_n(z) - R_{n-1}(z))} = \frac{A}{R_n(z) - z^2 R_{n-1}(z)} + \frac{B}{R_n(z) - R_{n-1}(z)}.$$

We can write $x_1 R_n(z) + y_1 R_{n-1}(z) = x_2 R_{n-1}(z) + y_2 R_{n-2}(z)$ where the coefficients are related to each other by the matrix equation:

$$\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = \begin{bmatrix} z^2 + 1 & 1 \\ -|a|^2 z^2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}.$$

Using an eigenvalue expansion, we find that:

$$\begin{aligned} R_{n-m}(z) &= (A + B)R_n(z) - (A + z^2 B)R_{n-1}(z) \\ &= \frac{1}{R_1(z)} [A(R_m(z) - R_{m-1}(z)) + B(R_m(z) - z^2 R_{m-1}(z))] R_{n-m+1}(z) \\ &\quad - \frac{|a|^2 z^2}{R_1(z)} [A(R_{m-1}(z) - R_{m-2}(z)) + B(R_{m-1}(z) - z^2 R_{m-2}(z))] R_{n-m}(z). \end{aligned}$$

By solving this system and using the result $R_m(z)^2 - R_{m+1}(z)R_{m-1}(z) = |a|^{2m} z^{2m} R_1(z)^2$, the result follows. \square

We are now ready to prove the main theorem of this section:

Theorem 3.7 *Let $R_n = R_n(1) = (1 + |b|)^n - (1 - |b|)^n$ and $B_n = (1 + |b|)^n + (1 - |b|)^n$.*

The following formulas hold:

$$P_n^{(m)}(1, 0) = \frac{|b|}{2} \left(\frac{R_{n-m}B_{m-1}}{B_{n-1}} \right), \quad P_n^{(m)}(0, 1) = 1 - \frac{|b|}{2} \left(\frac{B_{n-m-1}R_m}{B_{n-1}} \right)$$

$$H_n^{(m)} = -\frac{|b|}{2} \left(\frac{aB_{n-m-1}B_{m-1}}{bB_{n-1}} \right). \quad (3.38)$$

Proof: We may write the absorption probability as $P_n^{(m)}(1, 0) = \left(r_n^{(m)}(z) \odot \overline{r_n^{(m)}(\bar{z})} \right) (1)$. By combining proposition 3.5 and proposition 3.7, we find that there exists an $\epsilon > 0$ such that:

$$P_n^{(m)}(1, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{1}{z} r_n^{(m)}(z) \overline{r_n^{(m)}\left(\frac{1}{\bar{z}}\right)} dz.$$

Substituting the above lemmas into this equation, we may write:

$$P_n^{(m)}(1, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{|b|^2 |a|^{2m-2} z^{2m-1} R_{n-m}(z)^2}{(R_n(z) - z^2 R_{n-1}(z))(R_n(z) - R_{n-1}(z))} dz.$$

Using the partial fractions expansion from lemma 3.5, we may write:

$$P_n^{(m)}(1, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{|b|^2 z R_{n-m}(z)}{(1-z^2)R_1(z)} \left[\frac{R_m(z) - R_{m-1}(z)}{R_n(z) - R_{n-1}(z)} - \frac{R_m(z) - z^2 R_{m-1}(z)}{R_n(z) - z^2 R_{n-1}(z)} \right] dz.$$

By Lemma 3.2, the partial fraction on the right may be eliminated leading to the simplified expression:

$$P_n^{(m)}(1, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{|b|^2 z R_{n-m}(z)}{(z^2 - 1)R_1(z)} \left[\frac{R_m(z) - z^2 R_{m-1}(z)}{R_n(z) - z^2 R_{n-1}(z)} \right] dz.$$

The result follows from an application of the residue theorem as well as recognizing that $R_n - R_{n-1} = |b|B_{n-1}$. Calculation of $P_n^{(m)}(0, 1)$ and $H_n^{(m)}$ is similar. \square

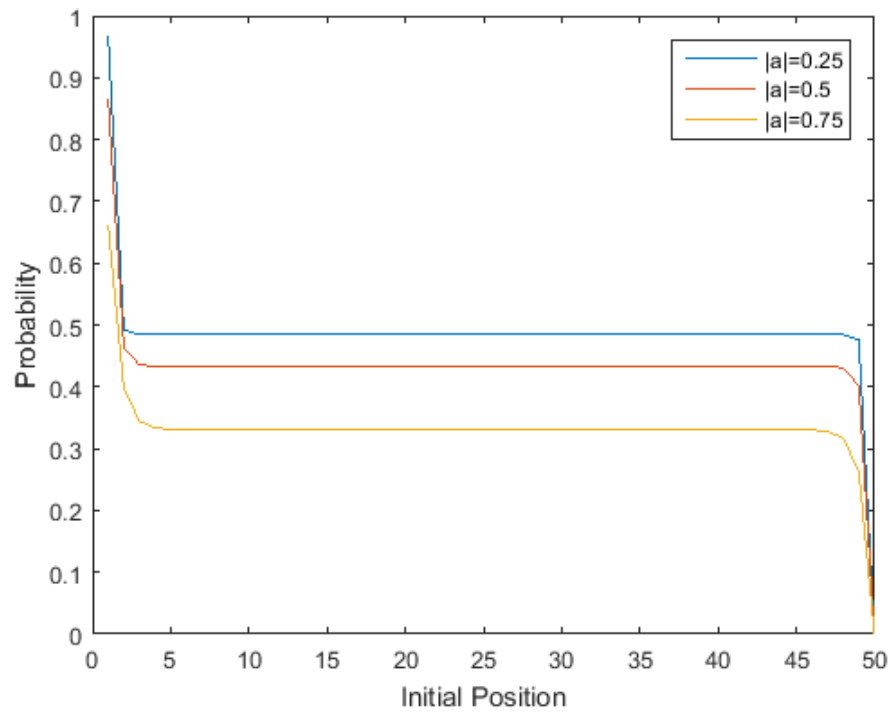


Figure 3.2: Plot of absorption probabilities $P_n^{(m)}(1, 0)$ for $n = 50$

Discussion

We note several differences between this quantum walk and the classical random walk. First, note that $P_\infty^{(1)}(\alpha, \beta) < 1$ unless $|\bar{b}\alpha + \bar{a}\beta| = 1$. This stands in contrast to the classical random walk which was recurrent in the symmetric case.

Second, the finite absorption probabilities do not limit to the semi-infinite absorption probabilities and this limit fails in a surprising way.

Theorem 3.8 *The following inequality is satisfied:*

$$P_\infty^{(1)}(\alpha, \beta) \leq P_n^{(1)}(\alpha, \beta). \quad (3.39)$$

Proof: By noting that a walk initialized in $|1\rangle(\alpha|R\rangle + \beta|L\rangle)$ will be absorbed at time $t = 1$ with probability $|\bar{b}\alpha + \bar{a}\beta|^2$ and will have a subsequent state of $(a\alpha + b\beta)|2\rangle|R\rangle$, we have:

$$P_n^{(1)}(\alpha, \beta) = 1 - \frac{|a\alpha + b\beta|^2}{|a|^2}(1 - P_n^{(1)}(1, 0)). \quad (3.40)$$

Thus, it suffices to prove this inequality for $P_n^{(1)}(1, 0)$. By using a trigonometric representation of the governing unitary matrix, proving this becomes equivalent to proving

$$f(\theta) = \pi \sin^3 \theta + 2\theta \cos 2\theta - \sin 2\theta \geq 0$$

where $\theta \in [0, \frac{\pi}{2}]$. The only values of θ in this interval such that $f'(\theta) = 0$ are $\theta \in \{0, \theta_0, \frac{\pi}{2}\}$ where $\theta_0 = \frac{3\pi}{8} \sin \theta_0$. It can be shown that $\frac{\pi}{4} < \theta_0$ and the result follows from noting that $f'(\frac{\pi}{4}) > 0$. \square

This is perhaps the most surprising result from the initial foray into absorption probabilities by Ambainis et. al. and here we have extended it to arbitrary internal state and arbitrary governing matrix. Not only do the finite probabilities fail to limit to the semi-infinite case, but the presence of an absorbing boundary sufficiently far to the right from the initial position will actually *increase* the probability of eventually being absorbed to

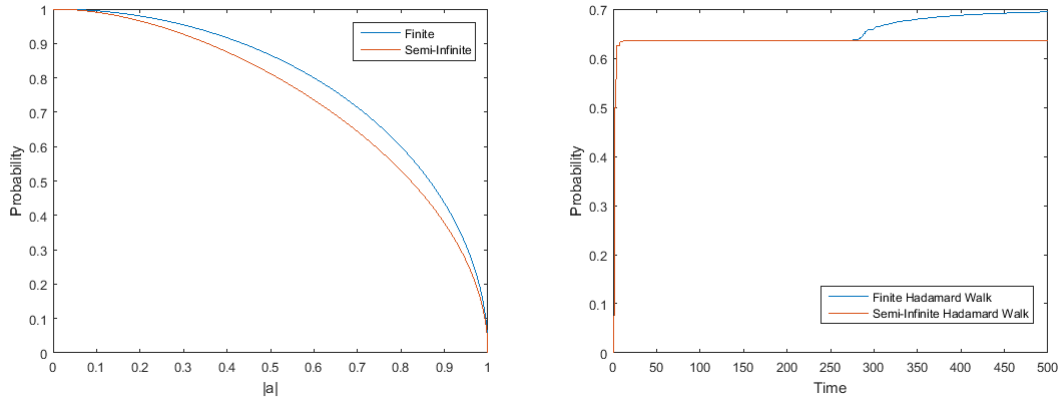


Figure 3.3: (*Left*) Comparison of absorption probabilities $P_\infty^{(1)}(1, 0)$ and $\lim_{n \rightarrow \infty} P_n^{(m)}(1, 0)$ (*Right*) Cumulative distribution function of the absorption probabilities $P_\infty^{(1)}(1, 0)$ and $P_n^{(1)}(1, 0)$ for $|a| = \frac{1}{\sqrt{2}}$ and $n = 100$

the left. This apparent paradox can be reconciled by considering the quantum walk to be a kind of discretization of the transport equation and that these absorbing boundaries do not necessarily absorb all information but reflects some as well. The figures below illustrate this concept. We present the following conjecture to extend this theorem:

Conjecture 3.1 *Theorem 3.8 is satisfied for arbitrary initial position m .*

We specify these limits in the finite case as we have in the classical random walk:

Theorem 3.9 *Let $0 < c < 1$. The following limiting probabilities hold:*

$$\lim_{n \rightarrow \infty} P_n^{(m)}(1, 0) = \frac{|b|}{2} \left[1 + \left(\frac{1 - |b|}{1 + |b|} \right)^{m-1} \right] \quad (3.41)$$

$$\lim_{n \rightarrow \infty} P_n^{(cn)}(1, 0) = \frac{|b|}{2}. \quad (3.42)$$

Another result which we display proves that the quantum walk particle in the finite absorption setting is guaranteed to eventually be absorbed by one of the boundaries:

Theorem 3.10 *The following formula holds:*

$$P_n^{(m)}(\alpha, \beta) + P_n^{(n-m)}(\beta, \alpha) = 1. \quad (3.43)$$

We conclude this section by proving two recurrences of these absorption probabilities:

Theorem 3.11 *The following recurrences hold for finite absorption probabilities:*

$$P_{n+1}^{(1)}(1, 0) = \frac{|b| + P_n^{(1)}(1, 0)}{1 + P_n^{(1)}(1, 0)} \quad (3.44)$$

$$P_n^{(m+3)}(\alpha, \beta) - \left(\frac{4}{|a|^2} - 1\right) P_n^{(m+2)}(\alpha, \beta) + \left(\frac{4}{|a|^2} - 1\right) P_n^{(m+1)}(\alpha, \beta) - P_n^{(m)}(\alpha, \beta) = 0. \quad (3.45)$$

Proof: The first equation can easily be proven true by recognizing that $\begin{bmatrix} R_{n+1} \\ B_{n+1} \end{bmatrix} = \begin{bmatrix} 1 & |b| \\ |b| & 1 \end{bmatrix}$. For the second equation, notice that $P_n^{(m)}$ is a linear combination of terms of the form $\{R_{n-m}B_m, R_{n-m}R_m, B_{n-m}B_m, B_{n-m}R_m\}$. If we let

$$V_m = [R_{n-m}B_m, R_{n-m}R_m, B_{n-m}B_m, B_{n-m}R_m]'$$

then the following equation holds:

$$V_{m+1} = \frac{1}{|a|^2} \begin{bmatrix} 1 & |b| & -|b| & -|b|^2 \\ |b| & 1 & -|b|^2 & -|b| \\ -|b| & -|b|^2 & 1 & |b| \\ -|b|^2 & -|b| & |b| & 1 \end{bmatrix} V_m.$$

The characteristic polynomial of this matrix is displayed as:

$$p(z) = (z - 1)^2 \left(z^2 + 2 \left(1 - \frac{2}{|a|^2} \right) z + 1 \right).$$

The conclusion follows from noting that the minimal polynomial retains only one of the factors of $(z - 1)$. \square

3.5 $(\mathbb{Z}, \tilde{C}_1, G_3)$ Quantum Walk

We repeat the analysis in the previous section for the $(\mathbb{Z}, \tilde{C}_1, G_3)$ quantum walk where $\tilde{C}_1 = \{-1, 0, 1\}$ and $G_3 = \frac{1}{3} \begin{bmatrix} -1 & 2 & 2 \\ 2 & -1 & 2 \\ 2 & 2 & -1 \end{bmatrix}$ is the 3×3 Grover matrix. This is also known as the three-state Grover walk and its unbounded behavior has been studied in several papers [37][27]. The three-state Grover walk exhibits a property known as *localization* in which the time averaged probability of observing the particle at its initial condition limits to a nonzero value. This is caused by the degeneration of eigenvalues in the Grover matrix and localization is exhibited for other quantum walks governed by Grover matrices [36].

These absorption probabilities have partially been computed in Wang et. al. [67] but we repeat the analysis here in a more concise framework. We refer back to the previous section for several of the proofs.

Semi-Infinite Case

In this section we aim to calculate absorption probabilities $P_\infty^{(m)}(\alpha, \beta, \gamma)$ or the probability that a particle initialized in $|m\rangle(\alpha|R\rangle + \beta|S\rangle + \gamma|L\rangle)$ is eventually absorbed in the $\Pi_{\text{no}}^0 Q \leftrightarrow (\mathbb{Z}, \tilde{C}_1, G_3, \{0\})$ absorbing quantum walk. Here, recognize that $T : |n\rangle|S\rangle \rightarrow |n\rangle|S\rangle$ for the translation operator associated with Q .

While the generalized absorption probability $P_\infty^{(m)}(\alpha, \beta)$ of the previous section depended only on the three quantities $P_\infty^{(m)}(1, 0)$, $P_\infty^{(m)}(0, 1)$, and $H_n^{(m)}$, these new absorption

probabilities depend on six such quantities. For illustrative purposes, we will only consider $P_\infty^{(m)}(1, 0, 0)$ as the others are computed via similar methods. We display the summation form of this probability:

$$P_\infty^{(m)}(1, 0, 0) = \sum_{t=1}^{\infty} |\langle 0, L|Q (\Pi_{\text{no}}^n Q)^{t-1} |m, R\rangle|^2.$$

In view of the summation form of the absorption probability, we construct the following generating function:

$$r_\infty^{(m)}(z) = \sum_{t=1}^{\infty} \langle 0, L|Q (\Pi_{\text{no}}^n Q)^{t-1} |m, R\rangle z^t.$$

We can define $l_\infty^{(m)}(z)$ and $s_\infty^{(m)}(z)$ similarly. We are thus interested in proving:

Proposition 3.9 *The generating function $r_\infty^{(m)}$ has the closed form:*

$$r_\infty^{(m)} = \left(\frac{3 + 2z + 3z^2 + (z-1)\sqrt{9+6z+9z^2}}{4z} \right) \left(\frac{-3 - 4z - 3z^2 + (z+1)\sqrt{9+6z+9z^2}}{2z} \right)^{m-1} \quad (3.46)$$

Proof: Note that the aforementioned generating functions are all segmented by $|m-1\rangle|L\rangle$. By using the segmenting transformation in conjunction with induction, this leads to the conclusion:

$$r_\infty^{(m)}(z) = r_\infty^{(1)}(z) \left(l_\infty^{(1)}(z) \right)^{m-1}.$$

It remains to handle the $m = 1$ generating functions. By combining a first step transformation and the previous equation, we have the system:

$$\begin{aligned} r_\infty^{(1)} &= \frac{2}{3}z + \frac{2}{3}zs_\infty^{(1)}(z) - \frac{1}{3}zr_\infty^{(1)}l_\infty^{(1)}(z) \\ s_\infty^{(1)} &= \frac{2}{3}z - \frac{1}{3}zs_\infty^{(1)}(z) + \frac{2}{3}zr_\infty^{(1)}l_\infty^{(1)}(z) \\ l_\infty^{(1)} &= -\frac{1}{3}z + \frac{2}{3}zs_\infty^{(1)}(z) + \frac{2}{3}zr_\infty^{(1)}l_\infty^{(1)}(z). \end{aligned} \quad (3.47)$$

Solving this system and choosing the root with a convergent Taylor series leads to the formula in the proposition. \square

Recognizing that $P_\infty^{(m)}(1, 0, 0) = \left(r_\infty^{(m)}(z) \odot \overline{r_\infty^{(m)}(\bar{z})} \right) (1)$, it remains to compute the Hadamard product. For the $m = 1$ case, we resort to direct integration.

Theorem 3.12 *The following holds:*

$$P_\infty^{(1)}(1, 0, 0) = \frac{5\sqrt{2}}{2\pi} - \frac{3 \csc^{-1}(3)}{4\pi} - \frac{3}{8} \approx 0.6693. \quad (3.48)$$

Finite Case

We now compute the absorption probability $P_n^{(m)}(1, 0, 0)$ for the absorbing quantum walk $\Pi_{\text{no}}^n \Pi_{\text{no}}^0 Q \leftrightarrow (\mathbb{Z}, \tilde{C}_1, G_3, \{0, n\})$. As before, the right absorption probability may be written as:

$$P_n^{(m)}(1, 0, 0) = \sum_{t=1}^{\infty} |\langle 0, L|Q (\Pi_{\text{no}}^n \Pi_{\text{no}}^n Q)^{t-1} |m, R\rangle|^2.$$

We thus construct generating functions $r_n^{(m)}(z)$ which have the form:

$$r_n^{(m)} = \sum_{t=1}^{\infty} \langle 0, L|Q (\Pi_{\text{no}}^n \Pi_{\text{no}}^n Q)^{t-1} |m, R\rangle z^t.$$

The generating functions $l_n^{(m)}(z)$ and $s_n^{(m)}(z)$ are constructed similarly. We compute closed form representations of these functions:

Proposition 3.10 *The following holds:*

$$r_n^{(m)}(z) = 2(z+1)(z-1)^{m-1} z^m \left(\frac{R_{n-m}(z)}{R_n(z) + z^2(1+3z)R_{n-1}(z)} \right) \quad (3.49)$$

$$l_n^{(m)}(z) = (z-1)^m z^m \left(\frac{R_{n-m}(z) + z^2(1+3z)R_{n-m-1}(z)}{R_n(z) + z^2(1+3z)R_{n-1}(z)} \right). \quad (3.50)$$

Here, $R_n(z) = \lambda_+(z)^n - \lambda_-(z)^n$ and

$$\lambda_{\pm}(z) = \frac{1}{2} \left[3 + z - z^2 - 3z^3 \pm \sqrt{(3 + z - z^2 - 3z^3)^2 - 4z^2(z-1)^2} \right].$$

Proof: Using the segmenting transformation, we find that

$r_n^{(m)}(z) = r_{n-m+1}^{(1)}(z) \prod_{k=2}^m l_{n-m+k}^{(1)}(z)$ and $l_n^{(m)}(z) = \prod_{k=1}^m l_{n-m+k}^{(1)}(z)$, and by the first step transformation we arrive at the following system:

$$\begin{aligned} r_n^{(1)} &= \frac{2}{3}z + \frac{2}{3}zs_n^{(1)}(z) - \frac{1}{3}zr_{n-1}^{(1)}l_n^{(1)}(z) \\ s_n^{(1)} &= \frac{2}{3}z - \frac{1}{3}zs_n^{(1)}(z) + \frac{2}{3}zr_{n-1}^{(1)}l_n^{(1)}(z) \\ l_n^{(1)} &= -\frac{1}{3}z + \frac{2}{3}zs_n^{(1)}(z) + \frac{2}{3}zr_{n-1}^{(1)}l_n^{(1)}(z). \end{aligned} \tag{3.51}$$

Solving this system gives us the following recursion:

$$r_{n+1}^{(1)}(z) = \frac{-z^2(1+3z)r_n^{(1)}(z) + 2z(z+1)}{-2z(z+1)r_n^{(1)}(z) + (z+3)}.$$

An appeal to the discussion in chapter 2 gives us the following closed form for $r_n^{(1)}(z)$:

$$r_n^{(1)}(z) = \frac{2z(z+1)R_{n-1}(z)}{R_n(z) + z^2(1+3z)R_{n-1}(z)}$$

Plugging this back into the system we can also solve for $l_n^{(1)}(z)$:

$$l_n^{(1)}(z) = z(z-1) \left(\frac{R_{n-1}(z) + z^2(1+3z)R_{n-2}(z)}{R_n(z) + z^2(1+3z)R_{n-1}(z)} \right).$$

Induction gives us the final result. □

We now wish to compute the Hadamard products of these generating functions. To do this, we will require a few lemmas.

Lemma 3.6 *Let $f(w, z) = \frac{-z^2(1+3z)w+2z(z+1)}{-2z(z+1)w+(z+3)}$. Then $|w|, |z| \leq 1 \Rightarrow |f(w, z)| \leq 1$.*

Proof: Notice that we may write $f(w, z) = z^3 \frac{b(z)}{b(\frac{1}{z})} \frac{-w+a(z)}{-a(\frac{1}{z})w+1}$ where $a(z) = \frac{2z(z+1)}{z^2(1+3z)}$ and

$b(z) = z^2(1 + 3z)$. The proof proceeds in the same way as did the proof of Lemma 4.1. \square

We also state the following two lemmas which aid in our calculations:

Lemma 3.7 *The following formulas hold:*

$$\overline{r_n^{(m)} \left(\frac{1}{z} \right)} = -2(z+1)(z-1)^{m-1} z^m \left[\frac{R_{n-m}(z)}{R_n(z) - (z+3)R_{n-1}(z)} \right] \quad (3.52)$$

$$\overline{l_n^{(m)} \left(\frac{1}{z} \right)} = (1-z)^m z^m \left[\frac{R_{n-m}(z) - (z+3)R_{n-m-1}(z)}{R_n(z) - (z+3)R_{n-1}(z)} \right]. \quad (3.53)$$

Lemma 3.8 *The following formula holds:*

$$\begin{aligned} & \frac{R_{n-m}(z)}{(R_n(z) + z^2(1+3z)R_{n-1}(z))(R_n(z) - (z+3)R_{n-1}(z))} \\ &= \frac{1}{(3+z+z^2+3z^3)z^{2m-2}(z-1)^{2m-2}R_1(z)} \left[\frac{R_m(z) - (z+3)R_{m-1}(z)}{R_n(z) - (z+3)R_{n-1}(z)} - \frac{R_m(z) + z^2(1+3z)R_{m-1}(z)}{R_n(z) + z^2(1+3z)R_{n-1}(z)} \right]. \end{aligned} \quad (3.54)$$

Proof: Let us assume this expression has a partial fractions form:

$$\begin{aligned} & \frac{R_{n-m}(z)}{(R_n(z) + z^2(1+3z)R_{n-1}(z))(R_n(z) - (z+3)R_{n-1}(z))} \\ &= \frac{A}{R_n(z) + z^2(1+3z)R_{n-1}(z)} + \frac{B}{R_n(z) - (z+3)R_{n-1}(z)}. \end{aligned}$$

Notice that if $x_1 R_{n+1}(z) + y_1 R_n(z) = x_2 R_n(z) + y_2 R_{n-1}(z)$, then we must have the following:

$$\begin{bmatrix} x_2 \\ y_2 \end{bmatrix} = \begin{bmatrix} 3+z-z^2-3z^3 & 1 \\ -z^2(z-1)^2 & 0 \end{bmatrix} \begin{bmatrix} x_1 \\ y_1 \end{bmatrix}.$$

The result follows from a similar argument to the result in lemma 3.5. \square

We are now ready to compute the absorption probabilities via the Hadamard product.

Theorem 3.13 *Let $\omega = \frac{1}{3} + \frac{2\sqrt{2}}{3}i$, $\delta_{\pm}(z) = \frac{1}{2} \left[-(3z^2 + 4z + 3) \pm \sqrt{(3z^2 + 4z + 3)^2 - 4z^2} \right]$, $F_n(z) = \delta_+(z)^n - \delta_-(z)^n$, and $B_n(z) = \delta_+(z)^n + \delta_-(z)^n$. Then the right absorption probability satisfies the following:*

$$P_n^{(m)}(1, 0, 0) = \frac{1}{2} \left[\frac{F_{n-m}(1)F_{m-1}(1)}{\sqrt{6}F_{m-1}(1)} - \frac{F_{n-m}(\omega)F_{m-1}(\omega)}{\sqrt{2}F_{m-1}(\omega)} \right]. \quad (3.55)$$

Proof: Using the Hadamard product integral representation and the partial fractions formula from lemma 3.8, there exists an $\epsilon > 0$ such that the following holds:

$$P_n^{(m)}(1, 0, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{4z(z+1)R_{n-m}(z)}{(3z^2 - 2z + 3)R_1(z)} \left[\frac{R_m(z) + z^2(1+3z)R_{m-1}(z)}{R_n + z^2(1+3z)R_{n-1}(z)} - \frac{R_m(z) - (z+3)R_{m-1}(z)}{R_n - (z+3)R_{n-1}(z)} \right] dz.$$

Lemma 3.1 gives us the following simplification:

$$P_n^{(m)}(1, 0, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{4z(z+1)R_{n-m}(z)}{(3z^2 - 2z + 3)R_1(z)} \left[\frac{R_m(z) + z^2(1+3z)R_{m-1}(z)}{R_n(z) + z^2(1+3z)R_{n-1}(z)} \right] dz.$$

Now recognize that we can write $\lambda_{\pm}(z) = \frac{z-1}{2} \left[-(3z^2 + 4z + 3) \pm \sqrt{(3z^2 + 4z + 3)^2 - 4z^2} \right]$. This allows us to write $R_n(z) = (z-1)^n F_n(z)$, and the integral may be rewritten in terms of these $F_n(z)$ functions:

$$P_n^{(m)}(1, 0, 0) = \frac{1}{2\pi i} \int_{|z|=1+\epsilon} \frac{4z(z+1)F_{n-m}(z)}{(3z^2 - 2z + 3)(z-1)F_1(z)} \left[\frac{(z-1)F_m(z) + z^2(1+3z)F_{m-1}(z)}{(z-1)F_n(z) + z^2(1+3z)F_{n-1}(z)} \right] dz.$$

The integrand is a rational function with only three poles $\{\omega_{\pm}, 1\}$ ($\omega_{\pm} = \frac{1+2\sqrt{2}i}{3}$) lying inside the contour of integration. We now apply residue theorem to this integral. As a visual, we now write this integral out as a sum:

$$\begin{aligned} P_n^{(m)}(1, 0, 0) &= \frac{4\omega_+(\omega_+ + 1)F_{n-m}(\omega_+)}{3(\omega_+ - \omega_-)(\omega_+ - 1)F_1(\omega_+)} \left[\frac{(\omega_+ - 1)F_m(\omega_+) + \omega_+^2(1+3\omega_+)F_{m-1}(\omega_+)}{(\omega_+ - 1)F_n(\omega_+) + \omega_+^2(1+3\omega_+)F_{n-1}(\omega_+)} \right] \\ &+ \frac{4\omega_-(\omega_- + 1)F_{n-m}(\omega_-)}{3(\omega_- - \omega_+)(\omega_- - 1)F_1(\omega_-)} \left[\frac{(\omega_- - 1)F_m(\omega_-) + \omega_-^2(1+3\omega_-)F_{m-1}(\omega_-)}{(\omega_- - 1)F_n(\omega_-) + \omega_-^2(1+3\omega_-)F_{n-1}(\omega_-)} \right] \\ &+ \frac{8F_{n-m}(1)}{3(1 - \omega_+)(1 - \omega_-)F_1(1)} \left[\frac{F_{m-1}(1)}{F_{n-1}(1)} \right]. \end{aligned}$$

Let $\lambda_+(z)^n + \lambda_-(z)^n = (z-1)^n B_n(z)$ and recognize that $(z-1)F_n(z) + z^2(1+3z)F_{n-1}(z) = \frac{1}{2} [(z+1)(3z^2 - 2z + 3)F_{n-1} + F_1(z)B_1(z)]$. Recognize further that $F_n(\omega_-) = -(-\omega_-^3)^n F_n(\omega_+)$. These two identities lead to the first result. \square

We remark that unlike in the right absorption probabilities, there are additional residues of $z = -1$ in these integrals in the left absorption probabilities. Since $F_n(-1) = 0$, we must make the following observation to avoid indeterminate expressions:

$$\lim_{z \rightarrow -1} \frac{F_n(z)}{z+1} = (-1)^n 2n\sqrt{3}.$$

Discussion

In this three state quantum walk we observe much of the same behavior as we did in the two state quantum walk. For instance, the semi-infinite walk is not recurrent; that is, $P_\infty^{(1)}(1,0,0) < 1$. Also, as with the two state quantum walk, the finite absorption probability does not limit to the semi-infinite absorption probability:

$$P_\infty^{(1)}(1,0,0) < \lim_{n \rightarrow \infty} P_n^{(1)}(1,0,0). \quad (3.56)$$

It was proven in Wang et. al. [67] that the finite absorption probabilities for $m = 1$ satisfy the following recursion:

Theorem 3.14 *The following formula holds:*

$$P_{n+1}^{(1)}(1,0,0) = \frac{2 + 3P_n^{(1)}(1,0,0)}{3 + 4P_n^{(1)}(1,0,0)}. \quad (3.57)$$

However, a third order linear recursion in position will not hold for the absorption probabilities of these walks as the terms $F_{n-m}(\omega)B_{m-1}(\omega)$ and $F_{n-m}(1)F_{m-1}(1)$ separately satisfy third order recursions in m . We reconcile this observation in the following theorem:

Theorem 3.15 *Let $p_m = P_n^{(m)}(1, 0, 0)$. Then the following recursion holds:*

$$p_{m+6} - 134p_{m+5} + 3599p_{m+4} - 6932p_{m+3} + 3599p_{m+2} - 134p_{m+1} + p_m = 0 \quad (3.58)$$

Proof: First notice the following relationships hold:

$$\begin{aligned} F_{n+1}(1) &= -5F_n(1) + 2\sqrt{6}B_n(1), & F_{n+1}(\omega) &= -(1 + 2\sqrt{2}i)F_n(\omega) + \frac{2\sqrt{2} + 8i}{3}B_n(\omega) \\ B_{n+1}(1) &= 2\sqrt{6}F_n(1) - 5B_n(1), & B_{n+1}(\omega) &= \frac{2\sqrt{2} + 8i}{3}F_n(\omega) - (1 + 2\sqrt{2}i)B_n(\omega) \\ F_{n-1}(1) &= -5F_n(1) - 2\sqrt{6}B_n(1), & F_{n-1}(\omega) &= -(1 - 2\sqrt{2}i)F_n(\omega) - 6\sqrt{2}B_n(\omega) \end{aligned} \quad (3.59)$$

$$B_{n-1}(1) = -2\sqrt{6}F_n(1) - 5B_n(1), \quad B_{n-1}(\omega) = -6\sqrt{2}F_n(\omega) - (1 - 2\sqrt{2}i)B_n(\omega).$$

If we let V_m be the vector

$$\begin{aligned} V_m &= [F_{n-m}(1)F_m(1), F_{n-m}(1)B_m(1), B_{n-m}(1)F_m(1), B_{n-m}(1)B_m(1), \dots \\ &\dots, F_{n-m}(\omega)F_m(\omega), F_{n-m}(\omega)B_m(\omega), B_{n-m}(\omega)F_m(\omega), B_{n-m}(\omega)B_m(\omega)]' \end{aligned}$$

then the following equation holds:

$$V_{m+1} = \begin{bmatrix} 25 & -10\sqrt{6} & 10\sqrt{6} & -24 & 0 & 0 & 0 & 0 \\ -10\sqrt{6} & 25 & -24 & 10\sqrt{6} & 0 & 0 & 0 & 0 \\ 10\sqrt{6} & -24 & 25 & -10\sqrt{6} & 0 & 0 & 0 & 0 \\ -24 & 10\sqrt{6} & 25 & -10\sqrt{6} & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 9 & -6\sqrt{2} & 6(\sqrt{2} + 4i) & -8(1 + 2\sqrt{2}i) \\ 0 & 0 & 0 & 0 & -6\sqrt{2} & 9 & -8(1 + 2\sqrt{2}i) & 6(\sqrt{2} + 4i) \\ 0 & 0 & 0 & 0 & 6(\sqrt{2} + 4i) & -8(1 + 2\sqrt{2}i) & 9 & -6\sqrt{2} \\ 0 & 0 & 0 & 0 & -8(1 + 2\sqrt{2}i) & 6(\sqrt{2} + 4i) & -6\sqrt{2} & 9 \end{bmatrix} V_m. \quad (3.60)$$

The characteristic polynomial of this matrix is as follows:

$$p(\lambda) = (\lambda - 1)^4(\lambda^2 - 98\lambda + 1)(\lambda^2 - 34\lambda + 1).$$

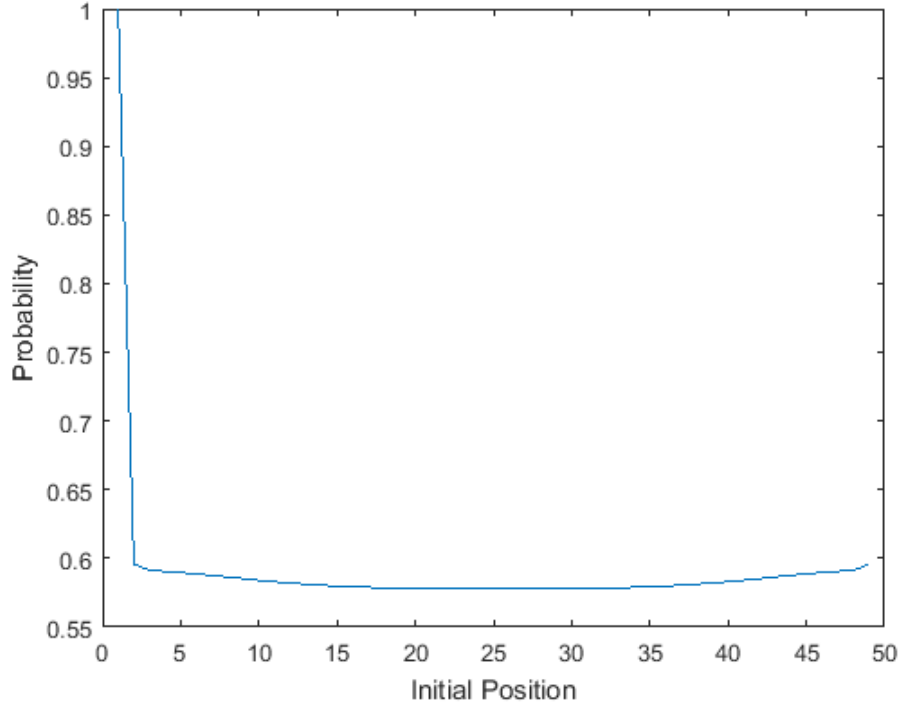


Figure 3.4: Plot of $P_n^{(m)}(1, 0, 0) + P_n^{(n-m)}(0, 0, 1)$ for $n = 50$

The theorem is proven by computing the minimal polynomial of this matrix. \square

A numerical analysis of these absorption probabilities illustrates the effects of localization on this system. In this case, below we show that unlike in the previous quantum walk, we have $P_n^{(m)}(1, 0, 0) + P_n^{(n-m)}(0, 0, 1) \leq 1$ where equality only holds when $m = 1$ or $m = n - 1$. This seems to support the idea that placing an absorbing boundary directly adjacent to an initialized particle will break down localization.

3.6 $(\mathbb{Z}^d, C_d, G_{2d})$ Quantum Walk

We now consider absorption probabilities for the $\Pi_{\text{no}}^{B_0} Q \leftrightarrow (\mathbb{Z}^d, C_d, G_{2d}, B_0)$ absorbing walk where $C_d = \{S_{\pm 1}, \dots, S_{\pm d}\}$ is the set of unit vectors in \mathbb{Z}^d , $B_k = \{z \in \mathbb{Z}^d : \varphi_1(z) = k\}$

where $\varphi_k : \mathbb{Z}^d \rightarrow \mathbb{Z}$ is a projection onto the k^{th} coordinate, and $G_{2d} = \frac{1}{d} \begin{bmatrix} 1 & \dots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \dots & 1 \end{bmatrix} - I_{2d}$ is the $2d \times 2d$ Grover matrix. We refer to B as an *absorbing wall*. We wish to calculate $P_\infty^{(m)}$, or the probability that the quantum walk particle initialized in $|(m, 0, \dots, 0)\rangle|S_{+1}\rangle$ is eventually absorbed by B . Here, $|S_{+1}\rangle$ represents the internal state which translates perpendicular away from the absorbing boundary. We write the absorption probability as follows:

$$P_\infty^{(m)} = \sum_{b \in B} \sum_{t=1}^{\infty} |\langle b, S_{-1} | Q(\Pi_{\text{no}}^{B_0} Q)^{t-1} |(m, 0, \dots, 0), S_{+1}\rangle|^2.$$

In this section, we will only consider this semi-infinite probabilities as the finite probabilities may be computed with similar methods as described previously.

In view of the summation form of the absorption probability, we construct the following generating functions:

$$f_{S_{\pm k}, x}^{(m)} = \sum_{t=1}^{\infty} \langle x, S_{-1} | Q(\Pi_{\text{no}}^{B_0} Q)^{t-1} |(m, 0, \dots, 0), S_{\pm k}\rangle z^t.$$

Here, $x \in B_0$. Solving closed form expressions for these generating functions is not as straightforward as it was in the one-dimensional walks, so instead of proving the closed form in one go, we opt to elucidate the process through a series of lemmas and propositions.

Lemma 3.9 *The following relation holds:*

$$f_{S_{\pm k}, x}^{(m)}(z) = \sum_{y \in B_0} f_{S_{\pm k}, y}^{(1)}(z) f_{S_{-1}, x-y}^{(m-1)}(z). \quad (3.61)$$

Proof: The result follows from noting that $f_{S_{\pm k}, x}^{(m)}(z)$ is segmented by B_{m-1} and conducting a segmenting transformation. \square

Lemma 3.10 *The following system is satisfied:*

$$f_{S_{\pm k}, x}^{(1)}(z) = \begin{cases} \left(\frac{1}{d} - \delta_{S_{-1}, S_{\pm k}} \right) z + \left(\frac{1}{d} - \delta_{S_{+1}, S_{\pm k}} \right) z f_{S_{+1}, x}^{(2)}(z) \\ + z \sum_{S \neq S_{\pm 1}} \left(\frac{1}{d} - \delta_{S, S_{\pm k}} \right) f_{S, x+S}^{(1)}(z) & x = 0. \\ \left(\frac{1}{d} - \delta_{S_{+1}, S_{\pm k}} \right) z f_{S_{+1}, x}^{(2)}(z) + z \sum_{S \neq S_{\pm 1}} \left(\frac{1}{d} - \delta_{S, S_{\pm k}} \right) f_{S, x+S}^{(1)}(z) & x \neq 0 \end{cases} \quad (3.62)$$

Proof: The result follows from a first step transformation and noting that if $x \neq 0$, the first step cannot be left. \square

The system of generating functions described by lemma 3.10 is infinite for $d \geq 2$. As such we need some sort of construction to reduce this infinite system to a finite one. Let us introduce the functions $F_{S_{\pm k}}^{(m)} : \mathbb{C} \times \mathbb{C}^d \rightarrow \mathbb{C}$ defined as follows:

$$F_{S_{\pm k}}^{(m)}(z, \Theta) = \sum_{x \in B_0} f_{S_{\pm k}, x}^{(m)}(z) e^{ix \cdot \Theta}.$$

Since $\varphi_1(x) = 0$ in this summation, we can informally think of $\Theta \in \mathbb{R}^{d-1}$ as opposed to \mathbb{R}^d . These new functions allow us to rewrite the previous lemmas to result in a finite system. We first reformulate the segmenting relation from lemma 3.9.

$$F_{S_{\pm k}}^{(m)}(z, \Theta) = F_{S_{\pm k}}^{(1)}(z, \Theta) \left(F_{S_{\pm k}}^{(1)}(z, \Theta) \right)^{m-1}.$$

We may now write the following system of $2d$ functions:

$$\begin{aligned} F_{S_{\pm k}}^{(1)}(z, \Theta) &= \left(\frac{1}{d} - \delta_{S_{-1}, S_{\pm k}} \right) z + \left(\frac{1}{d} - \delta_{S_{+1}, S_{\pm k}} \right) z F_{S_{+1}}^{(1)}(z, \Theta) F_{S_{-1}}^{(1)}(z, \Theta) \\ &+ z \sum_{S \neq S_{\pm 1}} \left(\frac{1}{d} - \delta_{S, S_{\pm k}} \right) e^{-iS \cdot \Theta} F_S^{(1)}(z, \Theta). \end{aligned}$$

If we solve this system, we now need a way to get back to the $f_{S_{\pm k}, x}^{(m)}(z)$ generating

functions. To do this, we take an inverse Fourier transform of $F_{S_{\pm k}}^{(1)}(z, \Theta)$:

$$f_{S_{\pm k}, x}^{(m)}(z) = \frac{1}{(2\pi)^d} \int_{\|\Theta\|_{\infty} \leq \pi} F_{S_{\pm k}}^{(m)}(z, \Theta) e^{ix \cdot \Theta} d\Theta.$$

Once we get back the f generating functions, we may compute the absorption probability via the usual Hadamard product technique:

$$P_{\infty}^{(m)} = \sum_{x \in B_0} \left(f_{S_{+1}, x}^{(m)}(z) \odot \overline{f_{S_{+1}, x}^{(m)}(\bar{z})} \right) (1).$$

These computations quickly become cumbersome even for $d = 2$, but with a computer algebra program an analytic representation for these absorption probabilities can be obtained.

3.7 Electric Quantum Walk

In this section we prove results on absorption probabilities of the electric quantum walk. The electric quantum walk [55] [20] is a space-inhomogeneous quantum walk named due to its similarity to a quantum mechanical system in the presence of an electric field. We define these walks as follows:

Definition 3.9 *Let $Q \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ be a quantum walk operator $Q = T(I \otimes U)$. We say that $Q_{\Theta} \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ is an electric quantum walk operator if $Q_{\Theta} = T(I \otimes e^{ix \cdot \Theta} U)$ where the coin is position dependent.*

The absorbing electric quantum walks may be defined similarly. In this section, we will compute the absorption probability $P(\theta)$ corresponding to the $\Pi_{\text{no}}^0 Q_{\theta} \leftrightarrow (\mathbb{Z}, C_1, U, \{0\})$ absorbing electric quantum walk parameterized by θ where the initial condition is $|1\rangle|R\rangle$.

We write this absorption probability in the form of equation (3.1):

$$P(\theta) = \sum_{t=1}^{\infty} |\langle 0, L | Q_{\theta} (\Pi_{\text{no}}^0 Q_{\theta})^{t-1} | 1, R \rangle|^2$$

In accordance with this summation form of the absorption probability, we define the generating function $r_\infty^{(m)}(z; \theta)$:

$$r_\infty^{(m)}(z; \theta) = \sum_{t=1}^{\infty} \langle 0, L | Q_\theta (\Pi_{\text{no}}^0 Q_\theta)^{t-1} | 1, R \rangle z^t$$

The function $l_\infty^{(m)}(z; \theta)$ is defined similarly.

The generating function $r_\infty^{(m)}(z; \theta)$ is segmented by $|m-1\rangle|L\rangle$. However, due to spatial inhomogeneity we must be cautious when writing the resulting relation. If $\gamma \in C_1^{m+1}$ is an n path from $|1\rangle|R\rangle$ to $|0\rangle|L\rangle$ and γ' is the same n path but from $|m\rangle|R\rangle$ to $|m-1\rangle|L\rangle$, then $A(\gamma') = e^{in(m-1)\theta} A(\gamma)$ since translational invariance no longer holds. As such, we can use induction and the segmenting relation to find:

$$r_\infty^{(m)}(z; \theta) = r_\infty^{(1)}(e^{i(m-1)\theta} z; \theta) \prod_{k=2}^m l_\infty^{(1)}(e^{i(m-k)\theta} z; \theta)$$

This relation is similar for $l_\infty^{(m)}(z; \theta)$. Now using a first step transformation and plugging in this relation, we have:

$$r_\infty^{(1)}(z; \theta) = -\bar{b}e^{i\theta} z + ae^{i\theta} z r_\infty^{(1)}(e^{i\theta} z; \theta) l_\infty^{(1)}(z; \theta)$$

$$l_\infty^{(1)}(z; \theta) = \bar{a}e^{i\theta} z + be^{i\theta} z r_\infty^{(1)}(e^{i\theta} z; \theta) l_\infty^{(1)}(z; \theta). \quad (3.63)$$

From these relations it is clear that $\theta \in 2\pi\mathbb{Q}$ will lead to a solvable system while we will need other methods to tackle this problem where $\theta \notin 2\pi\mathbb{Q}$. The dichotomy we have noted is pervasive in literature regarding the electric quantum walk. In particular, an electric quantum walk parameterized by $\theta \in 2\pi\mathbb{Q}$ will eventually become ballistic while a walk parameterized by $\theta \notin 2\pi\mathbb{Q}$ experiences some degree of Anderson localization. It is with this dichotomy in mind that we present the following conjecture:

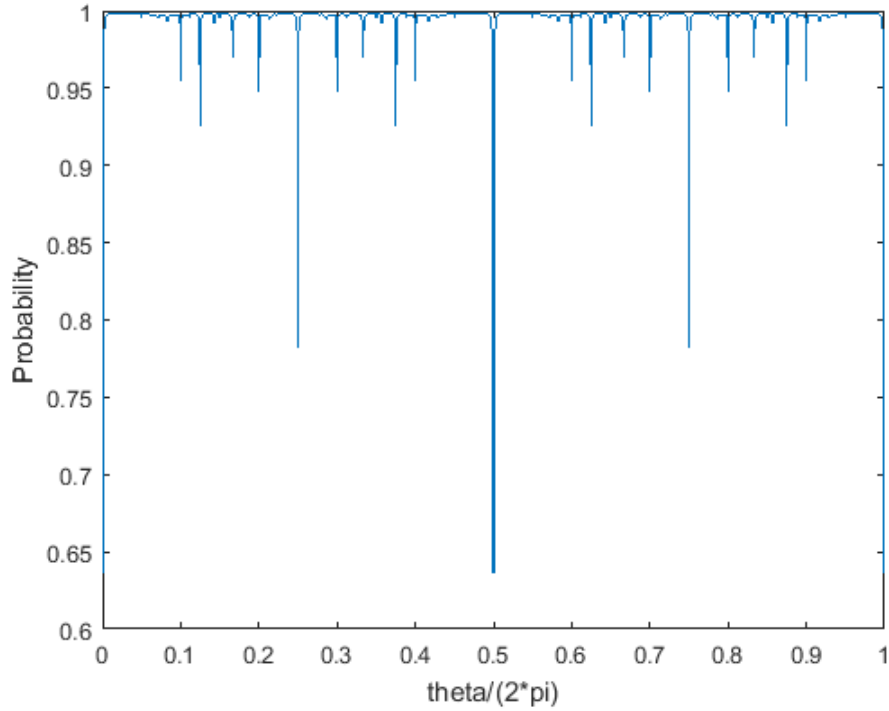


Figure 3.5: $P(\theta)$ for $|a| = \frac{1}{\sqrt{2}}$ where $\theta = 2\pi \frac{n}{100}$

Conjecture 3.2 Let $P(\theta)$ be defined as in EQN. Then $P(\theta) < 1$ for $\theta \in 2\pi\mathbb{Q}$ while $P(\theta) = 1$ for $\theta \notin 2\pi\mathbb{Q}$. Furthermore, if $\theta_1 = 2\pi \frac{p_1}{q_1}$ and $\theta_2 = 2\pi \frac{p_2}{q_2}$ are in lowest terms, then $q_1 > q_2 \Rightarrow P(\theta_1) < P(\theta_2)$.

It is likely that this result would not hold if the initial position of the particle was $|n\rangle$ where $n \geq 2$.

3.8 Conclusion

In this paper we have developed absorption probabilities for two and three state one dimensional quantum walks, and made partial progress toward computing absorption probabilities of electric quantum walks and higher dimensional quantum walks. In these examples we have found that the presence of an absorbing boundary far from the initial position of

the walker paradoxically increases the probability that the particle is absorbed at a near boundary. We resolve this phenomenon by considering that the quantum walk exhibits wavelike behavior and that information is reflected by an absorbing boundary. In addition, we have found two recursions which govern these absorption probabilities in both initial condition and boundary placement.

It is the hope of the author that these techniques may be extended to more general absorption settings. In particular, it would be interesting to compute absorption probabilities for a quantum walk in a d -dimensional absorbing box, or for a d -dimensional quantum walk with a single absorption unit at the origin. This result would require more sophisticated path counting arguments than the ones described above, but the procedure for computing the Hadamard product for the resulting generating functions would likely remain the same.

Chapter 4

Global Behavior of Finite Quantum Walks

Quantum walks are known to have nontrivial interactions with absorbing boundaries. In particular it has been shown that an absorbing boundary in the one dimensional quantum walk partially reflects information, as observed by computing absorption probabilities [9] [12]. In this paper, we shift our sights from the local phenomena of absorption probabilities to the global behavior of finite quantum walks. These systems may be represented by matrices, and thus long term behavior is given by the eigenvector corresponding to the top eigenvalue. In the finite absorbing random walk, these eigenvalues are predictably spaced on the interval $(-1, 1)$ and the corresponding eigenvectors are found to be finite samplings of sine functions. Meanwhile, the eigenvalues of the finite absorbing quantum walk accumulate on the unit circle and the corresponding top eigenvectors can only be estimated. We extend these results to quantum walks in two dimensions. In addition, these finite absorbing walks also have structure at smaller time scales in the form of modal phenomena, which we will computationally explore.

4.1 Introduction

The quantum walk is a unitary analogue of the classical random walk. Where classical random walks have been used in algorithms for classical computers [52] [25] [59] [26], quantum walks can be used in algorithms for quantum computers, providing various degrees of speedup over their classical counterparts [33] [22] [21] [7] [8]. As opposed to the random walk which spreads at $O(\sqrt{t})$, the quantum walk spreads at $O(t)$ and has highly oscillatory

behavior close to the wave fronts. The quantum walk has been studied in a variety of purely mathematical contexts as well [40] [65]. In this paper, we will explore the global behavior of finite quantum walks, both with and without absorbing boundaries.

Quantum walks with absorbing boundaries were first studied in the context of absorption probabilities. Let p_∞ be the probability that a Hadamard walk particle initialized in $|1\rangle|R\rangle$ is eventually absorbed at $|0\rangle$, and let p_n be the probability that this particle is absorbed at $|0\rangle$ in the presence of an additional absorbing boundary at $|n\rangle$. Ambainis et. al. [9] found that $p_\infty = \frac{2}{\pi}$ and $\lim_{n \rightarrow \infty} p_n = \frac{1}{\sqrt{2}}$. This paradoxical result seems to indicate that absorbing boundaries in the quantum walk partially reflect information. A sharper result was conjectured by these authors and later proved by Bach and Borisov [12] which states that $p_{n+1} = \frac{1+2p_n}{2+2p_n}$. These results were carried over to the three-state Grover walk as well [66]. Absorption probabilities are concerned with local behavior at an absorbing boundary as opposed to global behavior.

The quantum walk can be described as a linear combination of translations, so it is natural to view the quantum walk operator on a finite domain as a matrix. In the case of the quantum walk with absorbing boundaries, we can simply multiply the matrix associated with the quantum walk operator by a projection matrix which projects off of the absorbing boundaries. Questions of long term behavior of the quantum walk can thus be reduced to computing eigenvalues and eigenvectors of such a matrix. In particular, the long term behavior of a quantum walk is dominated by the eigenvector corresponding to the eigenvalue of largest absolute value. To compute the eigenvalues of a quantum walk matrix, we first calculate its characteristic polynomial $p_n(\lambda)$ where n is the size of the domain in question. These characteristic polynomials satisfy second order recursions which we exploit to compute the locations of the roots. Computation of the eigenvectors will be similar to the computation of these roots.

We perform this analysis on classical random walks as well as quantum walks for comparison. The characteristic polynomial of a classical random walk operator satisfies a Chebyshev recurrence. These recurrences admit simple trigonometric substitutions which

facilitate an exact description of the location of the eigenvalues [62]. With periodic boundaries, these eigenvalues are located on the closed interval $[-1, 1]$ while with absorbing boundaries the eigenvalues reside in the open interval $(-1, 1)$. This Chebyshev recurrence also governs the entries of the eigenvectors of the random walk, and we find that every eigenvector is a discrete sampling of a sine function of period k where the associated eigenvalue is the k^{th} largest of the set. This result is in line with the understanding of the classical random walk as a discretization of the heat equation, whose spectra is simply a continuation of the sets of eigenvalues we have listed here [45].

The global behavior of the finite quantum walk with periodic boundary conditions becomes relatively uninteresting to study once one realizes that the associated matrix is unitary. This implies that all eigenvalues of this matrix has absolute value 1, meaning that no steady state behavior emerges. However, it has been shown that the time averaged distribution of this quantum walk approaches a uniform distribution [4].

The global behavior of the finite quantum walk with absorbing boundaries is much more difficult to compute than its classical counterpart. The characteristic polynomial of the associated matrix does not satisfy such a neat recurrence, so we are forced to approximate the roots of this characteristic polynomial. We are able to prove that the eigenvalues uniformly approach the unit circle as the size of the domain increases. This implies that it takes much longer for the quantum walk to converge to a steady state than does the classical random walk. The eigenvectors corresponding to the top eigenvalues are numerically determined to be approximations of sine waves up to a phase. This implies that the probability distribution of the absorbing quantum walk will approach a squared sine wave in long time.

These absorbing quantum walks also contain structure on smaller time scales. Multiple times throughout the quantum walk, the probability distribution will localize about a variable number of evenly spaced locations in the domain. We refer to this behavior as *modal phenomena*. The mechanism behind this is yet unclear, but we analyze this computationally in a variety of settings.

The rest of the paper is organized as follows: section 4.2 is dedicated to defining the quantum walk and matrix representations of discrete processes. In section 4.3 we perform global analysis on finite walks with periodic boundary conditions and in chapter 4 we do the same for finite walks with absorbing boundaries. In section 4.5 we illustrate the modal phenomena in a variety of settings.

4.2 Definitions and Methods

To begin, we define the quantum walk on groups.

Definition 4.1 *Let (G, \cdot) be a group, let $\Sigma \subset G$ where $|\Sigma| = n$, and let $U \in U(n)$ where $U(n)$ is the set of $n \times n$ unitary matrices. The quantum walk operator $Q : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ corresponding to the triple (G, Σ, U) may be written as $Q = T(I \otimes U)$ where for $g \in G$ and $\sigma \in \Sigma$, $T : |g\rangle|\sigma\rangle \mapsto |g+\sigma\rangle|\sigma\rangle$. We denote this correspondence as $Q \leftrightarrow (G, \Sigma, U)$.*

The pair (G, Σ) can be thought of as an undirected Cayley graph which admits loops.

We must also define an absorbing quantum walk via measurement operators. Let $b \in G \times \Sigma$. The measurement operator $\Pi_{\text{yes}}^b : \ell^2(G \times \Sigma) \rightarrow \ell^2(G \times \Sigma)$ is a projection onto $|b\rangle$ while Π_{no}^b is a projection onto the subspace spanned by the states indexed by the elements of $G \setminus b$. The probabilistic interpretation of quantum mechanics dictates that if we measure a state $\psi \in \ell^2(G \times \Sigma)$ at $|b\rangle$, the resulting state becomes $\Pi_{\text{yes}}^b \psi$ with probability $\|\Pi_{\text{yes}}^b \psi\|^2$ and $\Pi_{\text{no}}^b \psi$ with probability $\|\Pi_{\text{no}}^b \psi\|^2$. If $B \subset G \times \Sigma$, let Π_{no}^B be the composition of no measurements for all $b \in B$. In this way, we can define the quantum walk operator for an absorbing quantum walk.

Definition 4.2 *Let $Q \leftrightarrow (G, \Sigma, U)$ be a quantum walk operator and let $B \subset G \times \Sigma$. Then we say that $\Pi_{\text{no}}^B Q$ is the absorbing quantum walk operator corresponding to the ordered quadruple (G, Σ, U, B) and we denote this correspondence as $\Pi_{\text{no}}^B Q \leftrightarrow (G, \Sigma, U, B)$.*

We use the no operator in our definition because if we observe the particle somewhere in B , then the experiment is terminated.

In this paper, we are interested in the computing the probability distribution of an absorbing quantum walk $\Pi_{\text{no}}^B Q \leftrightarrow (G, \Sigma, U, B)$ on $G \times \Sigma$ conditioned on the particle not being absorbed by B . If $\psi \in \ell^2(G \times \Sigma)$ is some initial condition, then we are interested in calculating the following function $P_t : G \times \Sigma \rightarrow [0, 1]$ for t large:

$$P_t(x) = \frac{|\langle x | (\Pi_{\text{no}}^B Q)^t | \psi \rangle|^2}{\sum_{x \in G \times \Sigma} |\langle x | (\Pi_{\text{no}}^B Q)^t | \psi \rangle|^2}. \quad (4.1)$$

However, for these absorbing quantum walks it is more natural to perform analysis on the probability amplitude spaces and then convert to the probability space.

The key realization is that if G is finite, we can represent the operators $Q \leftrightarrow (G, \Sigma, U)$ and $\Pi_{\text{no}}^B Q \leftrightarrow (G, \Sigma, U, B)$ as $|G| \cdot |\Sigma| \times |G| \cdot |\Sigma|$ matrices. Let Q be such a matrix with a set of eigenvalues $\Lambda = \{\lambda_1, \dots, \lambda_n\}$ and corresponding eigenvectors $V = \{v_1, \dots, v_n\}$ such that $Qv_k = \lambda_k v_k$. Define $S = \{k \in \{1, \dots, n\} : |\lambda_k| \geq |\lambda| \ \forall \lambda \in \Lambda\}$. If v' is an arbitrary vector with an eigenvector expansion $v' = \alpha_1 v_1 + \dots + \alpha_n v_n$, we can make the following approximation for t large:

$$Q^t v' = Q^t \left(\sum_{k=1}^n \alpha_k v_k \right) = \sum_{k=1}^n \alpha_k \lambda_k^t v_k = \sum_{k \in S} \alpha_k \lambda_k^t v_k + R(t).$$

Here, $R(t) = O(c^{-t})$ where $c < \frac{1}{|\Lambda|}$. Thus, to settle questions of long term behavior of these quantum walks we must calculate eigenvalues and eigenvectors of the corresponding matrices.

It will often occur that we need to take large powers of 2×2 matrices. Using an eigenvalue expansion, we derive:

Lemma 4.1 *Let $M = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$, $\lambda_{\pm} = \frac{1}{2} \left[a + d \pm \sqrt{(a+d)^2 - 4(ad-bc)} \right]$, and $F_n = \lambda_+^n - \lambda_-^n$. Then we have:*

$$M^n = \frac{1}{F_1} \begin{bmatrix} F_{n+1} - dF_n & bF_n \\ cF_n & F_{n+1} - aF_n \end{bmatrix}.$$

Furthermore, we have $F_{n+2} - (a + d)F_{n+1} + (ad - bc)F_n = 0$.

4.3 Finite Walks with Periodic Boundary Conditions

We begin our global analyses with finite walks with periodic boundary conditions. On the one-dimensional line, the periodic boundary conditions correspond to the quantum walk $Q \leftrightarrow (\mathbb{Z}/n\mathbb{Z}, \Sigma, U)$. On these walks, it is easier to iteratively compute the eigenvectors simultaneously with the eigenvalues rather than to calculate the characteristic polynomial outright. Spectral analysis of quantum walks on the circle have been considered in a few settings previously [69] [20].

Classical Random Walk

Let us first define the classical random walk:

Definition 4.3 *A classical random walk is a sequence of random variables $\{X_j\}_{j=0}^{\infty}$ which satisfy $P(X_{t+1} = X_t + 1) = p$ and $P(X_{t+1} = X_t - 1) = q = 1 - p$.*

On a one-dimensional lattice of length n with periodic boundary conditions, we may write the random walk operator R_n as an $n \times n$ matrix:

$$R_n = \begin{bmatrix} 0 & q & 0 & \dots & p \\ p & 0 & q & & \\ 0 & p & 0 & \ddots & \\ \vdots & & \ddots & \ddots & q \\ q & & & p & 0 \end{bmatrix}. \quad (4.2)$$

The set of eigenvalues is addressed by the following theorem:

Theorem 4.1 *Let Λ_n be the set of eigenvalues of R_n . This set may be written as follows:*

$$\Lambda_n = \{pe^{2\pi ik/n} + qe^{-2\pi ik/n} : k \in \{1, \dots, n\}\}. \quad (4.3)$$

Proof: It is easiest to begin by constructing an implied eigenvector of R_n . Let $v_k : \mathbb{C} \rightarrow \mathbb{R}$ such that $v(\lambda) = [v_1(\lambda), \dots, v_n(\lambda)]'$ is an eigenvector of R with eigenvalue λ . This implies the following formula must hold:

$$v_{k+1}(\lambda) = \frac{\lambda}{q}v_k(\lambda) - \frac{p}{q}v_{k-1}(\lambda).$$

Rewritten in matrix form, we have:

$$\begin{bmatrix} v_{k+1}(\lambda) \\ v_k(\lambda) \end{bmatrix} = \begin{bmatrix} \frac{\lambda}{q} & -\frac{p}{q} \\ 1 & 0 \end{bmatrix} \begin{bmatrix} v_k(\lambda) \\ v_{k-1}(\lambda) \end{bmatrix}.$$

Denote this multiplier matrix as M . Due to the periodic boundary conditions, we expect that $M^n \begin{bmatrix} v_1(\lambda) \\ v_n(\lambda) \end{bmatrix} = \begin{bmatrix} v_1(\lambda) \\ v_n(\lambda) \end{bmatrix}$. Using the results from lemma 4.1, we find that an eigenvalue λ must satisfy the following equation:

$$\frac{p}{q} \frac{F_n(\lambda)^2}{F_1(\lambda)^2} = \left(\frac{F_{n+1}(\lambda)}{F_1(\lambda)} - 1 \right) \left(1 + \frac{p}{q} \frac{F_{n-1}(\lambda)}{F_1(\lambda)} \right).$$

Here, $F_n(\lambda) = \omega_+(\lambda)^n - \omega_-(\lambda)^n$ and $\omega_{\pm}(\lambda) = \frac{1}{2q} \left[\lambda \pm \sqrt{\lambda^2 - 4pq} \right]$. Let $B_n(\lambda) = \omega_+(\lambda)^n + \omega_-(\lambda)^n$. By noticing that $F_n(\lambda)^2 - F_{n+1}(\lambda)F_{n-1}(\lambda) = \left(\frac{p}{q}\right)^{n-1} F_1(\lambda)^2$, $F_{n+1}(\lambda) = \frac{\lambda}{2q}F_n(\lambda) + \frac{F_1(\lambda)}{2}B_n(\lambda)$, and $\frac{p}{q}F_{n-1}(\lambda) = \frac{\lambda}{2q}F_n(\lambda) - \frac{F_1(\lambda)}{2}B_n(\lambda)$, we have the following equation:

$$B_n(\lambda) = \left(\frac{p}{q} \right)^n + 1.$$

We will use a trig substitution to solve for λ . To this end, let $\lambda(\theta) = 2\sqrt{pq} \cos \theta$ such that $B_n(\lambda(\theta)) = 2 \left(\sqrt{\frac{p}{q}} \right)^n \cos n\theta$. Solving for θ in the previous equation implies that $e^{i\theta} = \sqrt{\frac{p}{q}} e^{2\pi i k/n}$ for some $k \in \{1, \dots, n\}$. Substituting this into $\lambda(\theta)$ gives us the result. \square

Using similar methods will give us a representation of the corresponding eigenvectors of R_n :

Theorem 4.2 Let $V_k = [v_k(1), \dots, v_k(n)]'$ be an eigenvector of R_n with eigenvalue $pe^{2\pi ik/n} + qe^{-2\pi ik/n}$. Then the following formula holds:

$$v_k(x) = e^{-2\pi i x k/n}. \quad (4.4)$$

Proof: Let us normalize the eigenvector such that $v_k(n) = 1$ and $v_k(1) = a_k$. Again, let $F_n(\lambda) = \omega_+(\lambda)^n - \omega_-(\lambda)^n$ and $\omega_{\pm}(\lambda) = \frac{1}{2q} \left[\lambda \pm \sqrt{\lambda^2 - 4pq} \right]$. By the previous calculations, if λ_k is the eigenvalue associated with V_k , then $F_x(\lambda_k) = \left(\frac{p}{q}\right)^x e^{2\pi i x k/n} - e^{-2\pi i x k/n}$. The entries of the eigenvector may be written as follows:

$$v_k(x) = a_k \frac{F_x(\lambda_k)}{F_1(\lambda_k)} - \frac{p}{q} \frac{F_{x-1}(\lambda)}{F_1(\lambda)}. \quad (4.5)$$

Due to the periodic boundary conditions, a_k must satisfy the following:

$$a_k = a_k \frac{F_{n+1}(\lambda_k)}{F_1(\lambda_k)} - \frac{p}{q} \frac{F_n(\lambda)}{F_1(\lambda)}.$$

Solving this equation we find that $a_k = e^{-2\pi i k/n}$. Making this substitution into equation (5) gives us the result. \square

$(\mathbb{Z}/n\mathbb{Z}, C_1, U)$ Quantum Walk

We now perform a similar analysis on the $Q_n \leftrightarrow (\mathbb{Z}/n\mathbb{Z}, C_1, U)$ quantum walk where $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ is an arbitrary unitary matrix and $C_1 = \{1, n-1\} = \{R, L\}$. We consider the position space of this walk to be $\mathbb{Z}/n\mathbb{Z} = \{1, \dots, n\}$ so as to be consistent with the previous section. Let $\psi \in \ell^2(\mathbb{Z}/n\mathbb{Z} \times C_1)$ be represented as $\psi = [r_1, l_1, \dots, r_n, l_n]'$. We can

then write Q_n in matrix form as:

$$Q_n = \begin{bmatrix} 0 & U_- & 0 & \dots & U_+ \\ U_+ & 0 & U_- & & \\ 0 & U_+ & 0 & \ddots & \\ \vdots & & \ddots & \ddots & U_- \\ U_- & & & U_+ & 0 \end{bmatrix}. \quad (4.6)$$

$$\text{Here, } U_+ = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix} \text{ and } U_- = \begin{bmatrix} 0 & 0 \\ -\bar{b} & \bar{a} \end{bmatrix}.$$

Theorem 4.3 *If Λ_n is the set of eigenvalues of Q_n , then we may write the following:*

$$\Lambda_n = \{Re ae^{-2\pi ik/n} \pm i\sqrt{1 - (Re ae^{-2\pi ik/n})^2} : k \in \{1, \dots, n\}\}. \quad (4.7)$$

Proof: If $v(\lambda) = [r_1(\lambda), l_1(\lambda), \dots, r_n(\lambda), l_n(\lambda)]'$ is an eigenvector of Q_n with eigenvalue λ , then the following formulas must hold:

$$ar_k(\lambda) + bl_k(\lambda) = \lambda r_{k+1}(\lambda) \quad -\bar{b}r_k(\lambda) + \bar{a}l_k(\lambda) = \lambda l_{n-1}(\lambda).$$

Combining these formulas, we can write a matrix representation of the recurrence governing the entries of the eigenvector:

$$\begin{bmatrix} r_{n+1}(\lambda) \\ l_{n+1}(\lambda) \end{bmatrix} = \frac{1}{\lambda} \begin{bmatrix} a & b \\ \frac{a\bar{b}}{\bar{a}} & \frac{\lambda^2 + |b|^2}{\bar{a}} \end{bmatrix} \begin{bmatrix} r_n(\lambda) \\ l_n(\lambda) \end{bmatrix}.$$

If we let $\omega_{\pm}(\lambda) = \frac{1}{2} \left[\frac{\lambda^2+1}{a\lambda} \pm \sqrt{\left(\frac{\lambda^2+1}{a\lambda}\right)^2 - \frac{4a}{a}} \right]$ and $F_n(\lambda) = \omega_+(\lambda)^n - \omega_-(\lambda)^n$, then we can represent this in the following way:

$$\begin{bmatrix} r_k \\ l_k \end{bmatrix} = \frac{1}{F_1(\lambda)} \begin{bmatrix} \frac{a}{\lambda} F_k(\lambda) - \frac{a}{a} F_{k-1}(\lambda) & \frac{b}{\lambda} F_k(\lambda) \\ \frac{a\bar{b}}{a\lambda} F_k(\lambda) & F_{k+1}(\lambda) - \frac{a}{\lambda} F_k(\lambda) \end{bmatrix} \begin{bmatrix} r_n \\ l_n \end{bmatrix}.$$

Using the periodic boundary conditions, we find that the following equations must hold:

$$\frac{a|b|^2}{a\lambda^2} F_n(\lambda)^2 = \left(\frac{a}{\lambda} F_n(\lambda) - \frac{a}{a} F_{n-1}(\lambda) - F_1(\lambda) \right) \left(F_{n+1}(\lambda) - \frac{a}{\lambda} F_n(\lambda) - F_1(\lambda) \right).$$

By using the relationships $F_{n+1}(\lambda) = \left(\frac{\lambda^2+1}{2a\lambda} \right) F_n(\lambda) + \frac{1}{2} F_1(\lambda) B_n(\lambda)$ and $F_{n-1}(\lambda) = \frac{\bar{a}}{a} \left[\left(\frac{\lambda^2+1}{2a\lambda} \right) F_n(\lambda) - \frac{1}{2} F_1(\lambda) B_n(\lambda) \right]$ where $B_n(\lambda) = \omega_+(\lambda)^n + \omega_-(\lambda)^n$, we can simplify this equation to the following:

$$\omega_{\pm}(\lambda)^n = 1.$$

If we say that $\omega_{\pm}(\lambda_k) = e^{2\pi ik/n}$, then solving for λ_k gives us the result. \square

A similar method gives us a representation of the eigenvectors:

Theorem 4.4 *Let $v_{\pm k} = [r_{\pm k}(1), l_{\pm k}(1), \dots, r_{\pm k}(n), l_{\pm k}(n)]'$ be an eigenvector of Q_n corresponding to the eigenvalue:*

$$\lambda_{\pm k} = \operatorname{Re} a e^{-2\pi ik/n} \pm i \sqrt{1 - (\operatorname{Re} a e^{-2\pi ik/n})^2}. \quad (4.8)$$

Then we can write this eigenvector in the following form:

$$\begin{bmatrix} r_{\pm k}(x) \\ l_{\pm k}(x) \end{bmatrix} = \begin{bmatrix} 1 \\ \frac{\lambda_{\pm k} e^{2\pi ik/n} - a}{b} \end{bmatrix} e^{2\pi i x k/n}. \quad (4.9)$$

Proof: Let $F_n(\lambda)$ and $\omega_{\pm}(\lambda)$ be defined as they were previously. Since $\omega_+(\lambda_{\pm k}) = e^{2\pi ik/n}$,

we must have:

$$\omega_-(\lambda_{\pm k}) = \frac{\lambda_{\pm k}^2 + 1}{\bar{a}\lambda_{\pm k}} - e^{2\pi ik/n}.$$

By using the identity $\lambda_{+l}\lambda_{-k} = 1$ and rearranging terms, we find that $\omega_-(\lambda_{\pm k}) = \frac{a}{\bar{a}}e^{-2\pi ik/n}$.

Let $v_{\pm k} = [r_{\pm k}(1), l_{\pm k}(1), \dots, r_{\pm k}(n), l_{\pm k}(n)]$ be an eigenvector of Q_n with eigenvalue $\lambda_{\pm k}$ and let us normalize it such that $r_{\pm k}(n) = 1$. Using the periodic boundary conditions, we find that $l_{\pm k}(n)$ must satisfy the following:

$$l_{\pm k}(n) = \frac{F_1(\lambda_{\pm k}) - \frac{a}{\lambda_{\pm k}}F_n(\lambda_{\pm k}) + \frac{a}{\bar{a}}F_{n-1}(\lambda_{\pm k})}{\frac{b}{\lambda_{\pm k}}F_n(\lambda_{\pm k})}.$$

By expanding F in terms of ω_{\pm} , we can prove the following:

$$l_{\pm k}(n) = \frac{\lambda_{\pm k}e^{2\pi ik/n} - a}{b}$$

The result can thus be obtained using the previous representation of $r_{\pm k}(x)$ and $l_{\pm k}(x)$ and finessing the resulting expression. \square

4.4 Absorbing Finite Walks

We now discuss long term behavior of walks with absorbing boundaries. While in the previous two examples we constructed eigenvectors and used the periodic boundary conditions to compute the eigenvalues, in these absorbing walks it will be more suitable to calculate the characteristic function of the walk operator before computing the associated eigenvectors. This will be done not only to give a more complete picture of the spectra of these operators, but also because our previous method will break down in the quantum case.

Classical Random Walk

Let us consider a classical random walk on the set $\{1, \dots, n\}$ with absorbing boundaries at 1 and n ; that is, if the particle reaches one of these points, we terminate the walk. We

wish to find the probability distribution of the random walk particle conditioned on the particle not being absorbed. To do this, we consider the absorbing random walk operator R_n which may be represented as a $n \times n$ matrix in the following way:

$$R_n = \begin{bmatrix} 0 & q & 0 & \dots & 0 \\ p & 0 & q & & \\ 0 & p & 0 & \ddots & \\ \vdots & & \ddots & \ddots & q \\ 0 & & & p & 0 \end{bmatrix}. \quad (4.10)$$

We find that the characteristic function of this matrix satisfies the following recursion:

Proposition 4.1 *Let $p_n(\lambda) = \det(\lambda I - R_n)$. Then we have*

$$p_{n+1}(\lambda) = \lambda p_n(\lambda) - p q p_{n-1}(\lambda) \quad (4.11)$$

with $p_{-1}(\lambda) = 0$ and $p_0(\lambda) = 1$.

Armed with this recursive representation of the characteristic polynomials, we simply set $p_n(\lambda) = 0$ to solve for the eigenvalues of R_n . While we could easily note the connection between our characteristic polynomials and Chebyshev polynomials of the second kind [62], we opt to compute these roots explicitly so that we may understand how our method breaks down in the quantum case.

Theorem 4.5 *The set Λ_n consisting of the eigenvalues of R_n may be written as follows:*

$$\Lambda_n = \left\{ 2\sqrt{pq} \cos \frac{2\pi k}{n+1} : k \in \{1, \dots, n\} \right\} \quad (4.12)$$

Proof: We know that $p_n(\lambda) = 0 \Rightarrow \lambda \in \Lambda_n$. The characteristic polynomials satisfy the

following matrix identity:

$$\begin{bmatrix} p_{n+1}(\lambda) \\ p_n(\lambda) \end{bmatrix} = \begin{bmatrix} \lambda & -pq \\ 1 & 0 \end{bmatrix} \begin{bmatrix} p_n(\lambda) \\ p_{n-1}(\lambda) \end{bmatrix}.$$

An application of lemma 4.1 gives us the following closed form representation of $p_n(\lambda)$:

$$p_n(\lambda) = \frac{F_{n+1}(\lambda)}{F_1(\lambda)} \quad (4.13)$$

Here, $F_n(\lambda) = \omega_+(\lambda)^n - \omega_-(\lambda)^n$ and $\omega_{\pm}(\lambda) = \frac{1}{2} \left[\lambda \pm \sqrt{\lambda^2 - 4pq} \right]$. We now make the substitution $\lambda(\theta) = 2\sqrt{pq} \cos \theta$. Upon completing this substitution, we find $\omega_{\pm}(\lambda(\theta)) = \sqrt{pq} e^{\pm i\theta}$ and $F_n(\lambda(\theta)) = 2i (\sqrt{pq})^n \sin n\theta$. A substitution of this identity into equation (4.13) gives the following:

$$p_n(\lambda(\theta)) = (\sqrt{pq})^n \frac{\sin(n+1)\theta}{\sin \theta}. \quad (4.14)$$

The result follows from noting the n independent roots of this equation are located at $\theta = \frac{2\pi k}{n+1}$ where $k \in \{1, \dots, n\}$. \square

Notice that in comparison to the random walk with periodic boundary conditions, these absorbing random walks have purely real eigenvalues. Similar methods as used in the previous proof can be used to compute the corresponding eigenvectors.

Theorem 4.6 *Let $\lambda_k = 2\sqrt{pq} \cos \frac{2\pi k}{n+1}$ be an eigenvalue of R_n . Then the corresponding eigenvector $v_k = [v_k(1), \dots, v_k(n)]'$ satisfies the following:*

$$v_k(x) = \left(\sqrt{\frac{p}{q}} \right)^{x-1} \sin \left(\frac{2\pi kx}{n+1} \right) \quad (4.15)$$

Proof: For $1 < x < n$, the eigenvector v_k must satisfy the following formula:

$$pv_k(x-1) + qv_k(x+1) = \lambda_k v_k(x)$$

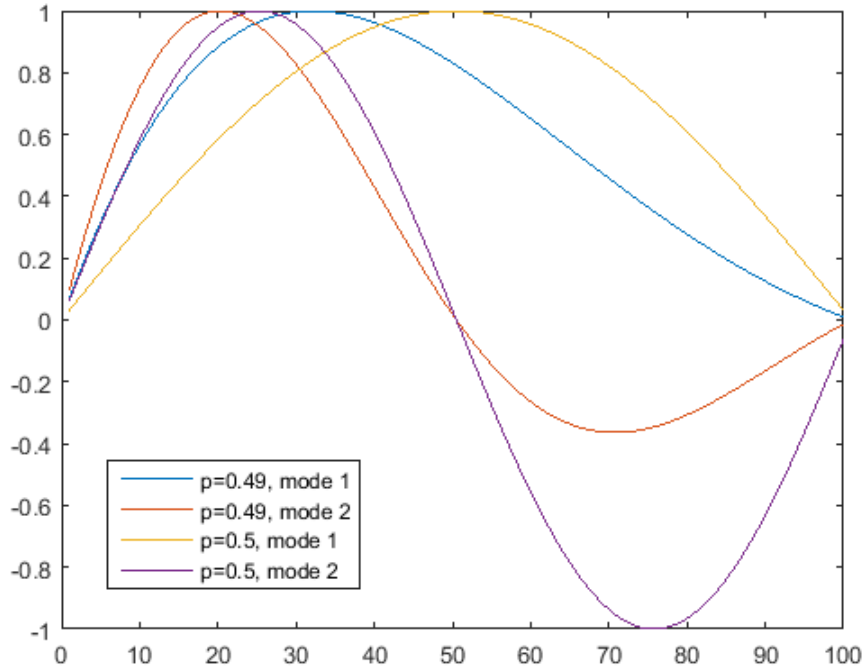


Figure 4.1: Top eigenvectors of the finite absorbing random walk operator R_n where $n = 100$

This equation constitutes a second order recursion amongst the entries of the eigenvector. We can normalize this eigenvector such that $v_k(1) = 1$ which implies that $v_k(2) = \frac{\lambda_k}{q}$. The solution follows by using lemma 3.1 and the previous trigonometric substitution. \square

We pause to note the similarity between the spectrum of the classical random walk and the spectrum of the heat equation [45]. More specifically, the spectrum of the classical random walk is a discrete sampling of the spectrum of the heat equation, just as the classical random walk itself is a discretization of the heat equation. We will find that we cannot compare the quantum walk to a continuous system in the same way.

$(\mathbb{Z}, C_1, U, \{1, n\})$ **Quantum Walk**

We now turn our attention to the $Q_n = \Pi_{\text{no}}^1 \Pi_{\text{no}}^n Q \leftrightarrow (\mathbb{Z}, C_1, U, \{1, n\})$ absorbing quantum walk where $C_1 = \{1, -1\} = \{R, L\}$ and $U = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ is a 2×2 unitary matrix. As in the random walk case, we can represent Q_n as a $2n \times 2n$ unitary matrix:

$$Q_n = \begin{bmatrix} 0 & U_- & 0 & \dots & 0 \\ U_+ & 0 & U_- & & \\ 0 & U_+ & 0 & \ddots & \\ \vdots & & \ddots & \ddots & U_- \\ 0 & & & U_+ & 0 \end{bmatrix}. \quad (4.16)$$

Here, let $U_+ = \begin{bmatrix} a & b \\ 0 & 0 \end{bmatrix}$ and let $U_- = \begin{bmatrix} 0 & 0 \\ c & d \end{bmatrix}$. To compute the eigenvalues of Q_n we first calculate the characteristic polynomial:

Proposition 4.2 *Let $p_n(\lambda) = \det(\lambda I - Q_n)$. These characteristic polynomials satisfy the following recursion:*

$$p_{n+1}(\lambda) = (\lambda^2 + ad - bc)p_n(\lambda) - ad\lambda^2 p_{n-1}(\lambda) \quad (4.17)$$

Here, $p_0(\lambda) = 1$ and $p_1(\lambda) = \lambda^2$.

We now specify our unitary matrix $U = \begin{bmatrix} a & b \\ -\bar{b} & \bar{a} \end{bmatrix}$ where $|a|^2 + |b|^2 = 1$. While in the classical random walk we were able to use a trig substitution to easily facilitate locating the eigenvalues, this procedure will not work here due to the initial conditions. The best we can do is to approximate the top few eigenvalues.

Theorem 4.7 *Let $\Theta_n = \{\theta \in \mathbb{C} : \sin n\theta = \pm i \frac{|a|}{|b|} \sin \theta, |\text{Re } \theta| < \pi\}$. Then the set Λ_n of*

eigenvalues of Q_n may be written as follows:

$$\Lambda_n = \{0\} \cup \{|a| \cos \theta \pm i\sqrt{1 - |a|^2 \cos^2 \theta} : \theta \in \Theta_n\}. \quad (4.18)$$

The eigenvalue $\lambda = 0$ has multiplicity 2.

Proof: Using lemma 4.1, we can derive a closed form for the characteristic polynomial:

$$p_n(\lambda) = \frac{\lambda^2}{F_1(\lambda)} [F_n(\lambda) - |a|^2 F_{n-1}(\lambda)]. \quad (4.19)$$

Here, $F_n(\lambda) = \omega_+(\lambda)^n - \omega_-(\lambda)^n$ and $\omega_{\pm}(\lambda) = \frac{1}{2} [\lambda^2 + 1 \pm \sqrt{(\lambda^2 + 1)^2 - 4|a|^2 \lambda^2}]$. This accounts for the eigenvalue at $\lambda = 0$ of multiplicity 2. Further manipulation of this expression implies that an eigenvalue λ of Q_n satisfies the following:

$$\frac{F_n(\lambda)}{B_n(\lambda)} = \frac{F_1(\lambda)}{2 - B_1(\lambda)}.$$

Here, $B_n(\lambda) = \omega_+(\lambda)^n + \omega_-(\lambda)^n$. We now consider the substitution $\lambda_{\pm}(\theta) = |a| \cos \theta \pm i\sqrt{1 - |a|^2 \cos^2 \theta}$. This leads to the restructuring of the previous expression as follows

$$\tan^2 n\theta = -\frac{|a|^2 \sin^2 \theta}{1 - |a|^2 \cos^2 \theta}$$

Further manipulating this expression in terms of strictly sine functions will give us the result. \square

This theorem diverges from the previous results involving eigenvalues in that these cannot be explicitly computed and depend on reference to a set such as Θ_n [32] [64] [15]. We provide an additional result to better visualize the location of the eigenvalues:

Proposition 4.3 *Let S_n be the set defined as follows:*

$$S_n = \{0\} \cup \{\lambda \in \mathbb{C} : |Re \lambda| < |a|, |Im \lambda| \geq |b|, r(n) < \lambda < 1\} \quad (4.20)$$

where $c(n) = \left(\frac{1+|a|}{1-|a|}\right)^{\frac{1}{2n}}$ and $r(n) = \frac{1}{2c(n)} \left[|a|(1-c(n)^2) \pm \sqrt{|a|^2(1-c(n)^2)^2 + 4c(n)^2}\right]$.
Then $\Lambda_n \subset S_n$.

Proof: Since Q_n does not increase the ℓ_2 norm of any state, it must follow that $\lambda \in \Lambda_n \Rightarrow |\lambda| \leq 1$. A simple calculation additionally shows that $\lambda \in \Lambda_n \Rightarrow |\lambda| < 1$. Suppose $p_n(\lambda) = 0$ and $\lambda \neq 0$. Then the following must hold:

$$\left| \frac{\omega_+(\lambda)}{\omega_-(\lambda)} \right|^n = \left| \frac{\omega_-(\lambda) - |a|^2}{\omega_+(\lambda) - |a|^2} \right|.$$

It is simple to show that $\left| \frac{\omega_-(\lambda) - |a|^2}{\omega_+(\lambda) - |a|^2} \right| \leq \frac{1+|a|}{1-|a|}$. If $|\lambda| = r$, then we also have that $\left| \frac{\omega_+(\lambda)}{\omega_-(\lambda)} \right| \geq \left(\frac{1-r^2 + \sqrt{(1-r^2)^2 + 4|a|^2 r^2}}{2|a|r} \right)^2$. \square

It should be noted that the eigenvalues of the absorbing quantum walk operator in some sense limit to the eigenvalues of the quantum walk operator on the circle. However, since the eigenvalues of the absorbing quantum walk all satisfy $|\lambda| < 1$, we find that the long term evolution drastically differs between the two quantum walks.

The eigenvectors must also be written with reference to the set Θ_n :

Theorem 4.8 *Let $v_k = [r_k(1), l_k(1), \dots, r_k(n), l_k(n)]'$ be an eigenvector of Q_n with eigenvalue λ_k where $\lambda_k = \lambda(\theta_k)$ with $\theta_k \in \Theta_n$ and $\lambda(\theta)$ defined as previously. If we let $\lambda_1 = \lambda_2 = 0$, then we have the following representation of eigenvectors:*

$$v_1 = [b, -a, 0, \dots, 0]', \quad v_2 = [0, \dots, 0, \bar{a}, \bar{b}]'$$

For $k > 2$, we have:

$$\begin{bmatrix} r_k(x) \\ l_k(x) \end{bmatrix} = \left(\frac{a}{|a|} \right)^x \begin{bmatrix} \bar{a}b \sin(x-1)\theta_k \\ |a|\lambda_k \sin x\theta_k - |a|^2 \sin(x-1)\theta_k \end{bmatrix}. \quad (4.21)$$

Proof: That $Q_n v_1 = Q_n v_2 = 0$ is trivial to check. We now handle the remaining eigenvectors. Each of these eigenvectors must satisfy $r_k(1) = 0$, and without loss of generality we

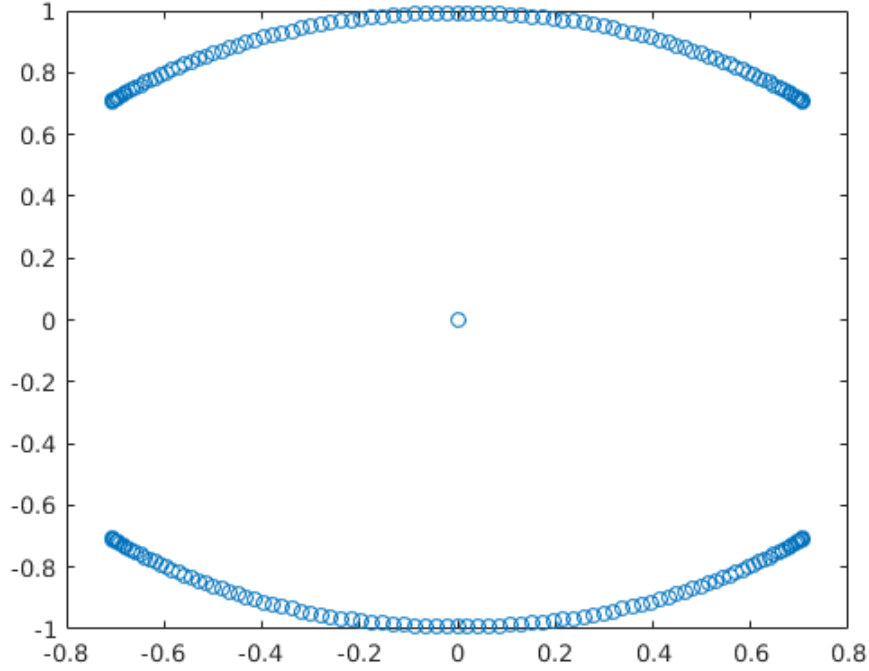


Figure 4.2: Eigenvalues for $\Pi_{n_0}^0 \Pi_{n_0}^n Q \leftrightarrow (\mathbb{Z}, C_1, H, \{0, n\})$ quantum walk operator in \mathbb{C}

can let $l_k(1) = 1$. As such, we can appeal to the proof of theorem 4.7 to find the following representation of the entries:

$$\begin{bmatrix} r_k(x) \\ l_k(x) \end{bmatrix} = \left(\frac{1}{\bar{a}\lambda_k} \right)^x \begin{bmatrix} \bar{a}bF_{x-1}(\lambda_k) \\ F_x(\lambda_k) - |a|^2F_{x-1}(\lambda_k) \end{bmatrix}.$$

Here, $F_n(\lambda)$ is defined how it was in the proof of Theorem 4.3. Using our previous representation of $F_x(\lambda(\theta_k)) = 2i(|a|\lambda(\theta_k))^x \sin x\theta_k$ gives us the result. \square

Numerical data indicates that for large n , the k^{th} top eigenvector is approximately a period $\frac{k}{2}$ sine function with position dependent phase. Important in this observation is that these modulus squared of these eigenvectors are independent of $|a|$. Thus, in large time, the probability distribution of the absorbing quantum walk approaches a squared sine function.

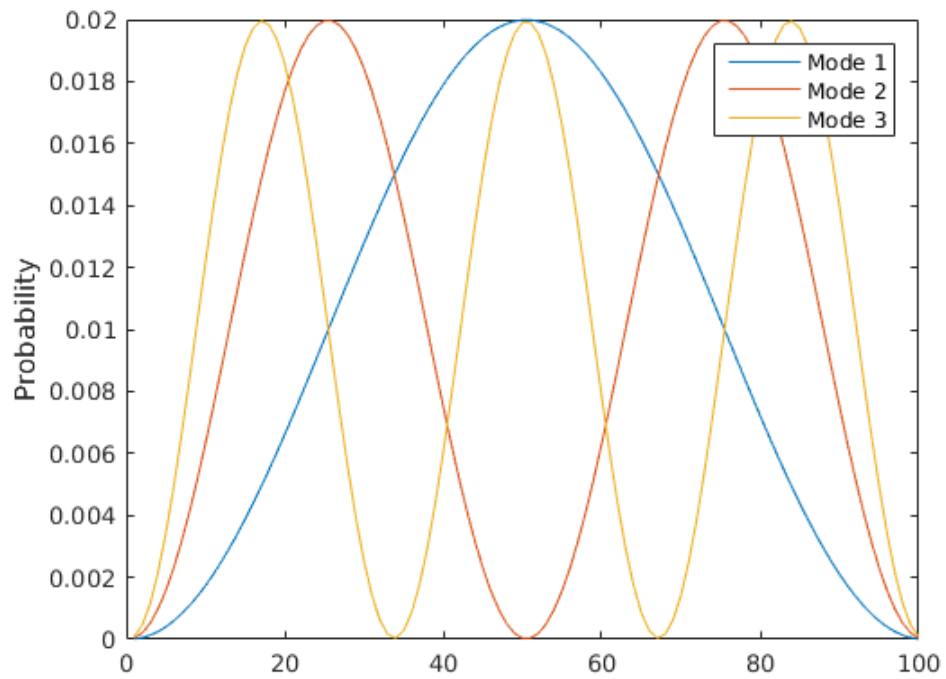


Figure 4.3: Top eigenvectors for the $Q_n = \Pi_{no}^0 \Pi_{no}^n Q \leftrightarrow (\mathbb{Z}, C_1, H, \{0, n\})$ absorbing walk operator displayed as conditional probability distributions where $n = 100$

We conclude this section by comparing these results to those on the classical random walk. There, we observed an intimate connection between the classical random walk and the heat equation; where the classical random walk is a discretization of the heat equation, the spectrum of the classical random walk is a discrete sampling of the spectrum of the heat equation with both boundary conditions. For the quantum walk, one can show that a similar continuation process will lead to a coupled wave equation [51]. If we attempt to impose absorbing boundaries on such an equation, we find that all energy is eventually dissipated. In this sense, we conclude that either this quantum walk is an inherently discrete process which cannot be properly explained by a continuous model, or the proper continuous model has not yet been found.

$(\mathbb{Z}, \tilde{C}_1, G_3, \{1, n\})$ **Quantum Walk**

We conduct an analysis similar to the one above for the $Q_n = \Pi_{\text{no}}^1 \Pi_{\text{no}}^n Q \leftrightarrow (\mathbb{Z}, \tilde{C}_1, G_3, \{1, n\})$ absorbing Grover walk. In this case, Q_n is a $3n \times 3n$ block tridiagonal matrix which may be displayed as follows:

$$Q_n = \begin{bmatrix} U_0 & U_- & 0 & \dots & 0 \\ U_+ & U_0 & U_- & & \\ 0 & U_+ & U_0 & \ddots & \\ \vdots & & \ddots & \ddots & U_- \\ 0 & & & U_+ & U_0 \end{bmatrix}. \quad (4.22)$$

Here, $U_+ = \frac{1}{3} \begin{bmatrix} -1 & 2 & 2 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$, $U_0 = \frac{1}{3} \begin{bmatrix} 0 & 0 & 0 \\ 2 & -1 & 2 \\ 0 & 0 & 0 \end{bmatrix}$, and $U_- = \frac{1}{3} \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 2 & 2 & -1 \end{bmatrix}$. We opt to compute the eigenvalues and eigenvectors of Q_n simultaneously by making use of the results from the previous section.

Theorem 4.9 Let Λ_n be the set of eigenvalues of Q_n and let Θ_n be the following set:

$$\Theta_n = \{\theta \in \mathbb{C} : \sin n\theta = \pm i \frac{1}{2} \sqrt{\frac{5 - \cos \theta}{1 + \cos \theta}} \sin \theta, |\operatorname{Re} \theta| < \pi\}. \quad (4.23)$$

Then we may write Λ_n as follows:

$$\Lambda_n = \{0, 1\} \cup \left\{ \frac{1}{3} \left[-2 + \cos \theta \pm i \sqrt{(5 - \cos \theta)(1 + \cos \theta)} \right] : \theta \in \Theta_n \right\} \quad (4.24)$$

Here, $\lambda = 0$ has multiplicity 2 and $\lambda = 1$ has multiplicity $n - 1$. Let

$v = [r(1), s(1), l(1), \dots, r(n), s(n), l(n)]'$ be an eigenvector of Q_n with corresponding eigenvalue $\lambda \in \Lambda_n$. If $\lambda = 0$, then we can write the two corresponding eigenvectors:

$$v = [2, 2, -1, 0, \dots, 0]'$$

$$v = [0, \dots, 0, -1, 2, 2]'. \quad (4.25)$$

If $\lambda = 1$, there exists a $1 \leq k < n$ such that the eigenvectors may be written as follows:

$$l(k) = r(k + 1) = 2, s(k) = s(k + 1) = 1 \quad (4.26)$$

If $\lambda \in \Lambda_n \setminus \{0, 1\}$ such that $\lambda = \frac{1}{3} \left[-2 + \cos \theta \pm i \sqrt{(5 - \cos \theta)(1 + \cos \theta)} \right]$, we can write the remaining eigenvectors as follows:

$$\begin{bmatrix} r(x) \\ s(x) \\ l(x) \end{bmatrix} = \begin{bmatrix} 2(\lambda + 1) \sin(x - 1)\theta \\ 2\lambda \sin x\theta + \sin(x - 1)\theta \\ \lambda(3\lambda + 1) \sin x\theta + (\lambda - 1) \sin(x - 1)\theta \end{bmatrix}. \quad (4.27)$$

Proof: From the construction of Q_n , an eigenvector v with eigenvalue λ must satisfy the following system:

$$-\frac{1}{3}r(x) + \frac{2}{3}s(x) + \frac{2}{3}l(x) = \lambda r(x + 1)$$

$$\frac{2}{3}r(x) - \frac{1}{3}s(x) + \frac{2}{3}l(x) = \lambda s(x) \quad (4.28)$$

$$\frac{2}{3}r(x) + \frac{2}{3}s(x) - \frac{1}{3}l(x) = \lambda l(x-1).$$

From the second equation, we have that $s(x) = \frac{2}{3\lambda+1}(r(x) + l(x))$, indicating that we need only consider the right and left internal states as the amplitude of the stationary internal state at a given position is a linear combination of the other internal states of that position. This reduction in system gives us the following:

$$-\frac{\lambda-1}{\lambda(3\lambda+1)}r(x) + \frac{2(\lambda+1)}{\lambda(3\lambda+1)}l(x) = r(x+1), \quad \frac{2(\lambda+1)}{\lambda(3\lambda+1)}r(x) + \frac{\lambda-1}{\lambda(3\lambda+1)}l(x) = l(x-1).$$

First, let us consider the eigenvalue $\lambda = 1$. This reduces the system to $l(x) = r(x+1)$, giving us the corresponding result found above.

For the remaining eigenvalues of Θ_n , we first rewrite the previous system in matrix form. Let $a = -\frac{\lambda-1}{\lambda(3\lambda+1)}$ and $b = \frac{2(\lambda+1)}{\lambda(3\lambda+1)}$. Then we have the following:

$$\begin{bmatrix} r(x+1) \\ l(x+1) \end{bmatrix} = \begin{bmatrix} a & b \\ -b & \frac{1-b^2}{a} \end{bmatrix} \begin{bmatrix} r(x) \\ l(x) \end{bmatrix}.$$

By lemma 4.1 and using the initial condition of $r(1) = 0$ and $l(1) = 1$, we write the following:

$$\begin{bmatrix} r(x) \\ l(x) \end{bmatrix} = \frac{1}{F_1} \begin{bmatrix} bF_{x-1} \\ F_x - aF_{x-1} \end{bmatrix}.$$

Here, $F_x = \omega_+^x - \omega_-^x$ and $\omega_{\pm} = \frac{1}{2a} \left[1 + a^2 - b^2 \pm \sqrt{(1 + a^2 - b^2)^2 - 4a^2} \right]$. A remaining eigenvalue $\lambda \in \Lambda_n$ must satisfy $F_x(\lambda) = a(\lambda)F_{x-1}(\lambda)$. Using the identities $F_{x+1} = \frac{1}{2} [B_1 F_x + F_1 B_x]$ and $B_x^2 - F_x^2 = 4$, we find that $F_x(\lambda) = \pm \frac{a(\lambda)}{b(\lambda)} F_1(\lambda)$. Upon substituting our previous values of a and b into this equation, we have the following:

$$\omega_{\pm}(\lambda) = -\frac{1}{2\lambda} \left[3\lambda^2 + 4\lambda + 3 \pm \sqrt{(3\lambda^2 + 4\lambda + 3)^2 - 4\lambda^2} \right].$$

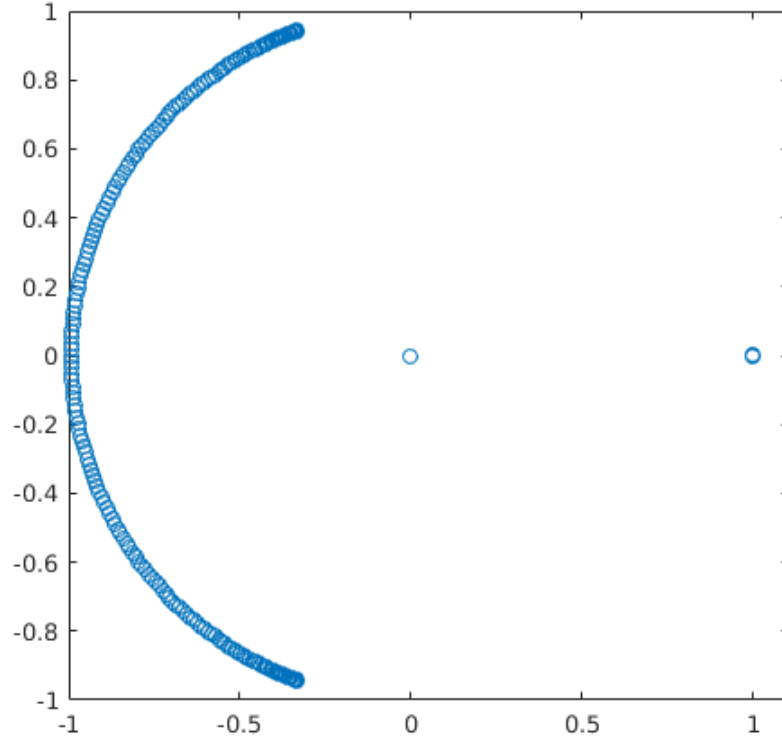


Figure 4.4: Location of eigenvalues for the $Q_n = \Pi_{\text{no}}^0 \Pi_{\text{no}}^n Q \leftrightarrow (\mathbb{Z}, \tilde{C}_1, G_3, \{0, n\})$ absorbing walk operator where $n = 100$

By making the substitution $\lambda(\theta) = \frac{1}{3} \left[-2 + \cos \theta \pm i \sqrt{(5 - \cos \theta)(1 + \cos \theta)} \right]$, we find that $F_n(\theta) = 2i \sin n\theta$ which accounts for Θ_n and the eigenvalues of Λ_n . Further substitutions give us the corresponding eigenvectors. \square

One may be interested in initializing the particle such that localization is not present in this walk. Konno et. al. stated that a walk initialized in $\Psi = \frac{1}{\sqrt{6}}|x\rangle [|R\rangle - 2|S\rangle + |L\rangle]$ does not exhibit localization. We can account for this by observing that Ψ is orthogonal to all of the eigenvectors with eigenvalue 1.

$(\mathbb{Z}^2, C_2, U, B_{X,Y})$ **Quantum Walk**

In this section we informally describe a procedure to construct eigenvectors of the two dimensional absorbing quantum walk operators $Q_{X,Y} = \Pi_{\text{no}}^{B_{X,Y}} Q \leftrightarrow (\mathbb{Z}^2, C_2, U, B_{X,Y})$. We define the *absorbing box* $B_{X,Y}$ as follows:

$$B_{X,Y} = \{(x, y) \in \mathbb{Z}^2 : x = 1 \text{ or } x = X \text{ or } y = 1 \text{ or } y = Y\}. \quad (4.29)$$

While $Q_{X,Y}$ may be represented as a $4XY \times 4XY$ unitary matrix, it is in general difficult to compute the characteristic polynomial outright due to its large size. As such, we opt to construct an eigenvector directly and make inferences about the corresponding eigenvectors.

Let $v = \{r_{x,y}, l_{x,y}, u_{x,y}, d_{x,y}\}_{x \leq X, y \leq Y}$ be an eigenvector of $Q_{X,Y}$ with eigenvalue λ . The entries of v must satisfy the following four way recursion:

$$Uv_{x,y} = \lambda[r_{x+1,y}, l_{x-1,y}, u_{x,y+1}, d_{x,y-1}]'$$

The naive hope may be to construct matrices $M_x(\lambda)$ and $M_y(\lambda)$ such that $M_x(\lambda)v_{x,y} = v_{x+1,y}$ and $M_y(\lambda)v_{x,y} = v_{x,y+1}$. However, this is impossible due to the lack of information given by the recursion. For example, there are only two equations relating $v_{x,y}$ and $v_{x+1,y}$ and if $v_{x,y}$ is known, there are four unknowns in $v_{x+1,y}$. Thus, we must be more subtle in regards to how we proceed with computing these eigenvectors.

Let $\lambda \neq 0$. Then we expect that $u_{x,1} = 0$, $r_{1,y} = 0$, $d_{x,Y} = 0$, and $l_{X,y} = 0$. In general, we will be working from left to right and bottom to top. In the one dimensional case, we were able to normalize the eigenvector such that $l_1 = 1$ and proceed down the line with matrix multiplications. However, we cannot normalize our eigenvector right away because we will need to assume values in a few entries to compute the rest of the eigenvector. To this end, let us assume values $l_{1,k} = y_k$ and $d_{k,1} = x_k$. With these values, we "know" six of the eight values in $v_{1,1}$ and $v_{2,1}$ with $r_{2,1}$ and $l_{2,1}$ being unknown. As mentioned before, we have two equations relating $v_{1,1}$ and $v_{2,1}$, thus the two unknowns can be written in terms

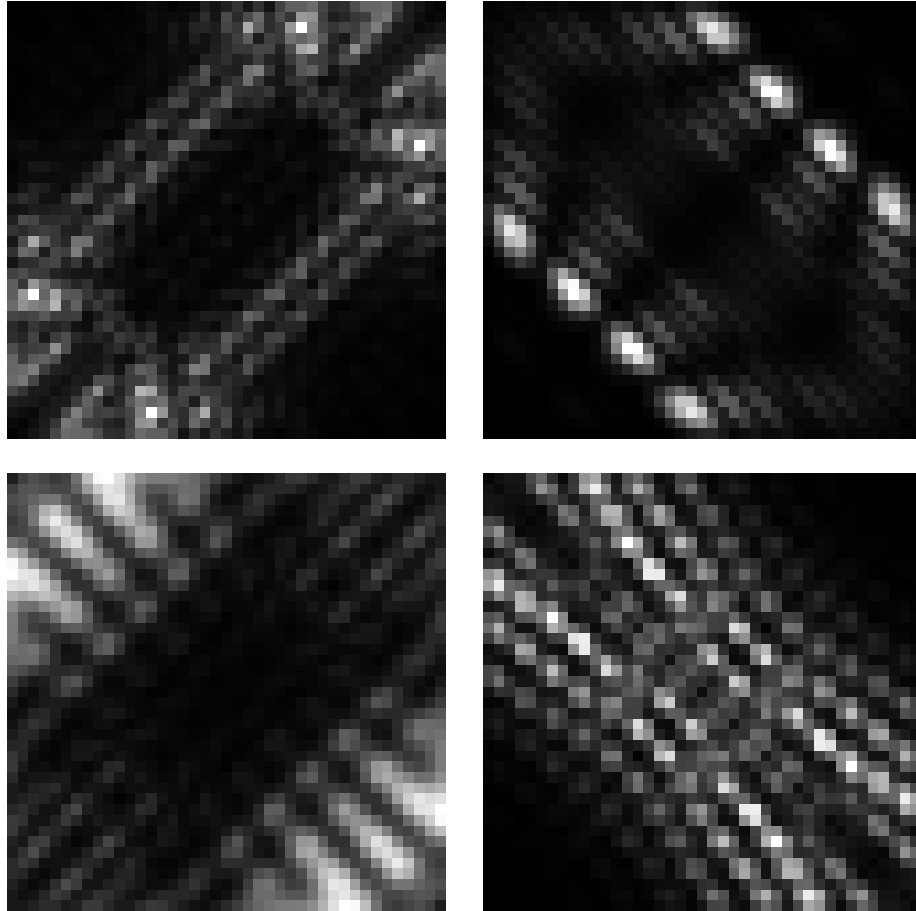


Figure 4.5: Eigenvalues of the $Q_{X,Y} = \Pi_{\text{no}}^{B_{X,Y}} Q \leftrightarrow (\mathbb{Z}^2, C_2, H \otimes H, B_{X,Y})$ absorbing walk operator displayed as conditional probability distributions where $X = Y = 41$

of y_1 , x_1 , and x_2 . We continue iteratively across this first row relating $r_{k,1}$ and $l_{k,1}$ to y_1 and $\{x_j\}_{j \leq k}$ until we arrive at $v_{X,1}$. Here, we find $r_{1,X}$ as a function of the aforementioned variables, however since $l_{X,1} = 0$, there exists a linear function $F(y_1, x_1, \dots, x_X) = 0$ which can be manipulated to represent y_1 in terms of x_1, \dots, x_X . We can now move from $v_{1,1}$ to $v_{1,2}$ using the same technique as before but now relating $u_{1,2}$ and $d_{1,2}$ to y_2 and $\{x_k\}_{k \leq X}$. Since $v_{1,2}$ and $v_{2,1}$ are accounted for, we can solve for $v_{2,2}$ as there are four equations and four unknowns. Proceeding in this way across the row, we may again solve for y_2 in terms of x_1, \dots, x_X . Extending this allows us to solve for y_k in terms of x_1, \dots, x_X up to $k = Y - 1$. In regards to $v_{1,Y}$, we can solve for $u_{1,Y}$ in terms of y_Y and x_1, \dots, x_X , but since $d_{1,Y} = 0$, we can represent y_Y in terms of x_1, \dots, x_X . Working across the top row, we find that since $d_{k,Y} = 0$, we can represent x_{X-k+2} in terms of x_1, \dots, x_{X-k+1} . Eventually, we will be able to write $a(\lambda)x_1 = x_2$ where $a(\lambda)$ is a rational function. By recognizing that $l_{X,Y} = 0$, we will find an additional equation $b(\lambda)x_1 = x_2$ such that the eigenvalues of $Q_{X,Y}$ must satisfy $a(\lambda) = b(\lambda)$.

We illustrate this procedure for the $\Pi_{\text{no}}^{B_{X,Y}} Q \leftrightarrow (\mathbb{Z}^2, C_2, G_4, B_{X,Y})$ quantum walk. On the bottom row, we have $u_{x,1} = 0$ and $r_{1,1} = 0$. Using the left and right relations from the Grover matrix, we have the following system:

$$r_{x+1,1} = -\frac{1}{2\lambda}r_{x,1} + \frac{1}{2\lambda}l_{x,1} + \frac{1}{2\lambda}d_{x,1}, \quad l_{x,1} = -\frac{1}{2\lambda}r_{x,1} + \left(\frac{1}{2\lambda} - 2\lambda\right)l_{x,1} + \frac{1}{2\lambda}d_{x,1} + d_{x+1,1}.$$

We want to describe $r_{x,1}$ and $l_{x,1}$ in a linear combination of $d_{1,1}, \dots, d_{x,1}$ and $l_{1,1}$. Let $x_k = d_{k,1}$ and let $y_1 = l_{1,1}$ such that we can write the following:

$$r_{n,1} = a_n y_1 + \sum_{k=1}^n b_{k,n} x_k, \quad l_{n,1} = c_n y_1 + \sum_{k=1}^n e_{k,n} x_k.$$

Using the two previous recursions and recognizing that $a_1 = 0$ and $c_1 = 1$, we may write

the following:

$$\begin{bmatrix} a_n \\ c_n \end{bmatrix} = \begin{bmatrix} -\frac{1}{2\lambda} & \frac{1}{2\lambda} \\ -\frac{1}{2\lambda} & \frac{1}{2\lambda} - 2\lambda \end{bmatrix}^{n-1} \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Applying lemma 4.1 to this equation gives us the following:

$$a_n = \frac{F_{n-1}(\lambda)}{2\lambda F_1(\lambda)}, \quad c_n = -\frac{F_{n+1}(\lambda)}{2\lambda F_1(\lambda)}.$$

Here, $F_n(\lambda) = \omega_+(\lambda)^n - \omega_-(\lambda)^n$ and $\omega_{\pm}(\lambda) = -\lambda \pm i\sqrt{1-\lambda^2}$. In regards to the other coefficients, notice that $b_{k,j} = 0$ for $k \geq j$ and $e_{k,j} = 0$ for $k > j$. Furthermore, we must have $e_{k,k} = 1$, $b_{k-1,k} = \frac{1}{\lambda}$, and $e_{k-1,k} = \frac{1}{\lambda} - 2\lambda$. If $1 < k < n$, then the following holds:

$$\begin{bmatrix} b_{k,n+1} \\ e_{k,n+1} \end{bmatrix} = \begin{bmatrix} -\frac{1}{2\lambda} & \frac{1}{2\lambda} \\ -\frac{1}{2\lambda} & \frac{1}{2\lambda} - 2\lambda \end{bmatrix} = \begin{bmatrix} b_{k,n} \\ e_{k,n} \end{bmatrix}.$$

For the special case of $k = 1$, we can write the following expressions for the corresponding coefficients:

$$b_{1,n} = \frac{F_{n-1}(\lambda)}{2\lambda F_1(\lambda)}, \quad e_{1,n} = -\frac{F_{n+1}(\lambda)}{2\lambda F_1(\lambda)}$$

For $n > 2$ and $k > n$, we may write the following:

$$b_{k,n} = \frac{1}{\lambda F_1(\lambda)} [F_{n-k}(\lambda) + \lambda F_{n-k-1}(\lambda)], \quad e_{k,n} = \frac{1}{\lambda F_1(\lambda)} [(1 - 2\lambda^2)F_{n-k}(\lambda) - \lambda F_{n-k-1}(\lambda)].$$

From the boundary conditions, we must have that $l_{X,1} = 0$. As such, we can calculate $l_{1,1}$ as a linear combination of $\{d_{x,1}\}$:

$$l_{1,1} = d_{1,1} - \frac{2}{F_{X+1}(\lambda)} \sum_{k=2}^X [(1 - 2\lambda^2)F_{X-k}(\lambda) - \lambda F_{X-k-1}(\lambda)] d_{k,1}.$$

We can plug this back into our previous equations to find $r_{n,1}$ and $l_{n,1}$ as a linear combination of $\{d_{k,1}\}$. If we work our way up the rows of the lattice as described in the previous chapter, these expressions become unwieldy, however it still is possible to find an expression

whose roots are the eigenvalues of $Q_{X,Y}$.

As with the three state Grover walk in one dimension, it can be shown that localization is also present in this two dimensional Grover walk. In the previous section, we posited that localization in a quantum walk could be presented as the existence of eigenvalues with $|\lambda| = 1$ in the associated operator. This is possible in the (\mathbb{Z}^2, C_2, G_4) walk with the following states:

$$\frac{1}{2\sqrt{2}} [|x, y\rangle(|L\rangle + |D\rangle) + |x + 1, y\rangle(|R\rangle + |D\rangle) + |x, y + 1\rangle(|L\rangle + |U\rangle) + |x + 1, y + 1\rangle(|R\rangle + |U\rangle)]. \quad (4.30)$$

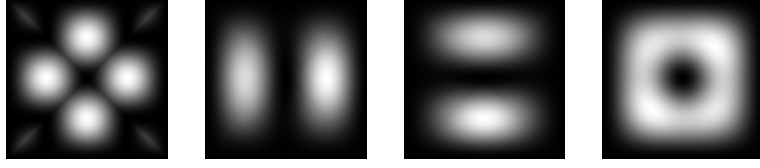
$(\mathbb{Z}^2, C_2, U, B_{X,Y} \cup \{(x, y)\})$ Quantum Walk

We now consider the finite two dimensional quantum walk with one defect, otherwise written as $\Pi_{\text{no}}^{B_{X,Y}} \Pi_{\text{no}}^{(x,y)} Q \leftrightarrow (\mathbb{Z}^2, C_2, U, B_{X,Y} \cup \{(x, y)\})$. In these walks, it is yet unclear how to compute the corresponding eigenvalues and eigenvectors. However, we display numerical simulations of a variety of these walks for large times. In particular, take an interest in the case $U = G_4$, which we term the non-localized Grover walk. By initializing the particle at the site of the defect, we remove localization and get a clearer picture of the lower eigenstates. We frame this observation as a conjecture:

Conjecture 4.1 *Consider the $Q_{X,Y} = \Pi_{\text{no}}^{B_{X,Y}} \Pi_{\text{no}}^{(0,0)} \leftrightarrow (\mathbb{Z}^2, C_2, G_4, B_{X,Y} \cup \{(\frac{X}{2}, \frac{Y}{2})\})$ quantum walk operator and let $\Psi = |(\frac{X}{2}, \frac{Y}{2})\rangle (\alpha|R\rangle + \beta|L\rangle + \gamma|U\rangle + \delta|D\rangle)$ be the initial condition. Let $A(\Psi)$ be the time-averaged distribution defined as follows:*

$$A(\Psi) = \lim_{T \rightarrow \infty} \frac{1}{T} \sum_{t=1}^{\infty} \frac{|Q_{X,Y}^t \Psi|^2}{\|Q_{X,Y}^t \Psi\|^2}. \quad (4.31)$$

For $X = Y$ sufficiently large, $A(\Psi)$ will limit to one of the four probability distributions below.

Figure 4.6: Conjectured distributions of $A(\Psi)$

Electric Quantum Walk

Before concluding this section, we briefly introduce the electric quantum walk [55] [20] and computationally explore how spatial inhomogeneities can alter the spectrum of the quantum walk. The electric quantum walk, named for its similarity to conducting a quantum walk in an electric field, is defined as follows:

Definition 4.4 *Let $Q \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ be a quantum walk operator $Q = T(I \otimes U)$. We say that $Q_\Theta \leftrightarrow (\mathbb{Z}^d, \Sigma, U)$ is an electric quantum walk operator if $Q_\Theta = T(I \otimes e^{ix \cdot \Theta} U)$ where the unitary coin is position dependent.*

The absorbing electric quantum walk is defined similarly.

The spatial inhomogeneity of the electric quantum walk gives us a slightly different recursion governing the characteristic polynomials of its matrix representation.

Proposition 4.4 *Let $Q_n(\theta) = \Pi_{n_0}^1 \Pi_{n_0}^n Q_\theta \leftrightarrow (\mathbb{Z}, C_1, U, \{1, n\})$ be an absorbing quantum walk operator and let $p_n(\lambda)$ be the characteristic polynomial of $Q_n(\theta)$. Then $p_n(\lambda)$ satisfies the following functional equation:*

$$p_n(\lambda) = \left(\lambda^2 e^{i(2n-2)\theta} + e^{i(2n+1)\theta} \right) p_{n-1} \left(\frac{\lambda}{e^{i\theta}} \right) - \lambda^2 e^{i(4n-5)\theta} |a|^2 p_{n-2} \left(\frac{\lambda}{e^{2i\theta}} \right). \quad (4.32)$$

As stated by previous literature on electric quantum walks, there is significant difference between the cases $\theta \in 2\pi\mathbb{Q}$ and $\theta \notin 2\pi\mathbb{Q}$. For $\theta = 2\pi\frac{p}{q}$ where $p, q \in \mathbb{N}$, it is possible to find a closed form for $p_n(\lambda)$. We observe that the eigenvectors of $Q_n(\theta)$ are similar to those in the analogous two-state standard quantum walk but in some sense divided into blocks of

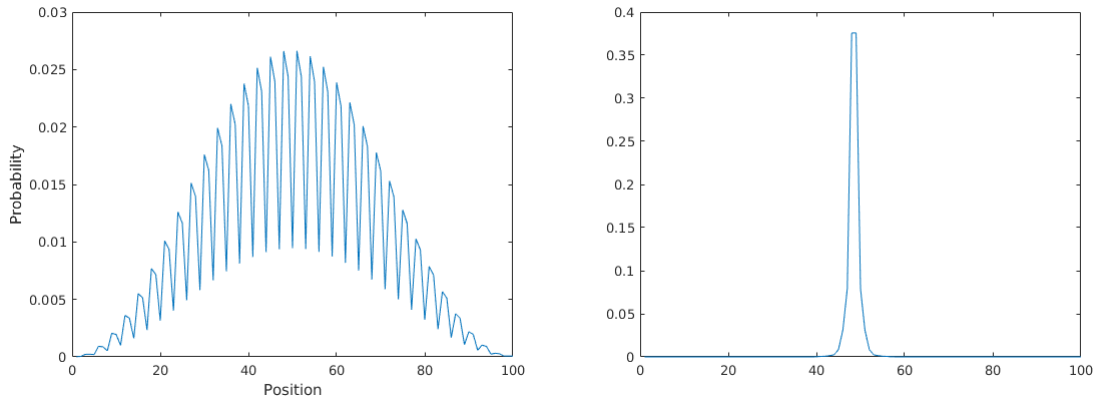


Figure 4.7: (*Left*) Eigenvector of an electric quantum walk with $\theta = \frac{2\pi}{3}$ (*Right*) Typical eigenvector of an electric quantum walk with $\theta \notin 2\pi\mathbb{Q}$.

size q . For $\theta \notin 2\pi\mathbb{Q}$ the situation is much different. Though precise computation of the eigenvalues and eigenvectors is out of reach due to the nature of this functional equation, we observe that a significant number of eigenvalues have absolute value very close to 1. We cite Cedzich et. al. and their description of revivals in these quantum walks as well as their connection to Anderson localization as a possible explanation of these numerical computations.

4.5 Modal Phenomena

Our previous discussion details the long term behavior of finite quantum walks. In particular, we noted that since the eigenvalues of an absorbing quantum walk operator limit uniformly to the unit circle, we expect that the emergence of a dominant eigenvector should take much longer than it would in the random walk case. In this section, we discuss the behavior of such quantum walks on smaller time scales. In particular, we document what we will refer to as *modal phenomena*, or the emergence of evenly spaced peaks in the probability distribution of the quantum walk at regular intervals.

Figure 8 displays the $(\mathbb{Z}, C_1, H, \{0, 200\})$ quantum walk (initialized at $|100\rangle|R$) at a variety of times during which these sharp peaks, or modes, emerge in the conditional

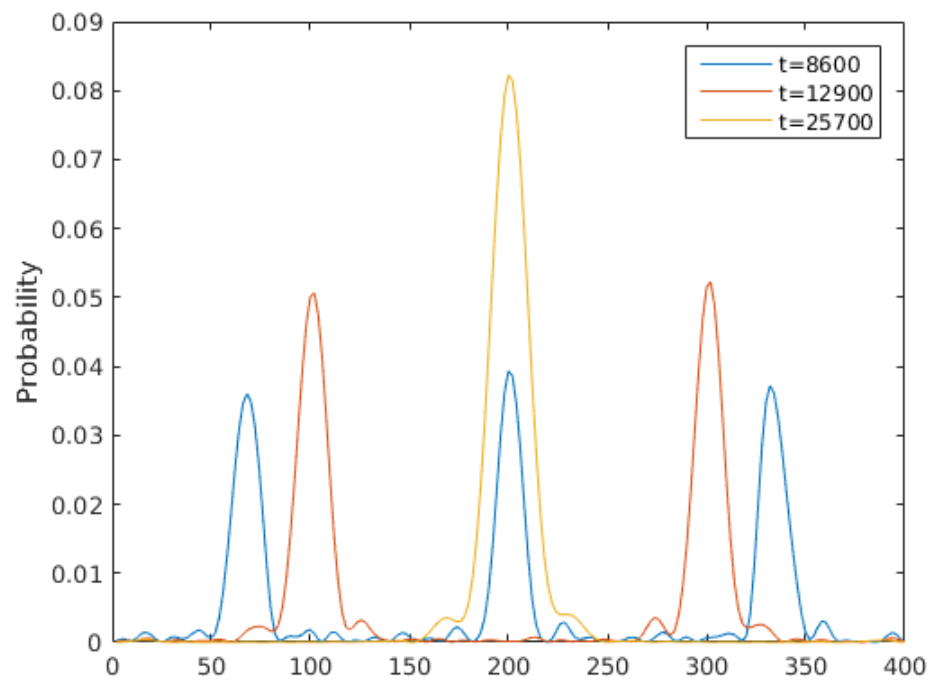


Figure 4.8: Conditional distribution of the $(\mathbb{Z}, C_1, H, \{0, n\})$ absorbing walk at various times

distribution. These modes are apparently equally spaced, equally sized, and appear in a variety of quantities. In an effort to describe the continual reappearance of these modes over time, we must find a quantity which describes how "modal" a conditional distribution is at a given time. For this task we opt to use entropy [23].

Definition 4.5 *Let $p : \Omega \rightarrow \mathbb{R}$ be a probability distribution. We define the entropy of this distribution to be the following:*

$$H(p) = - \sum_{\omega \in \Omega} p(\omega) \log p(\omega). \quad (4.33)$$

Intuitively, entropy is a measure of the uncertainty of a probability distribution. On this domain, the uniform distribution would maximize the entropy functional while a delta potential would minimize it. In the plot of entropy over time in Figure 9, we expect that the local minima occur at times for which modal distributions arise. These local minima are structured in a very precise way to suggest the following conjecture:

Conjecture 4.2 *Let $\Pi_{n_0}^0 \Pi_{n_0}^n Q \leftrightarrow (\mathbb{Z}, C_1, H, \{0, n\})$ be an absorbing quantum walk operator and let $p(\cdot, t)$ be the conditional probability distribution at time t given an initial condition $\Psi = |\frac{n}{2}\rangle |R\rangle$. There exists an N such that at time $t = \frac{p}{q}N$ where $\frac{p}{q}$ is in lowest terms and p and q are relatively small, the distribution $p(\cdot, t)$ will have q modes.*

It should be noted that modal phenomena has not been observed for general initial conditions. In Figure 9, it is shown that a random initial condition does not lead to any significant patterns in entropy over time. We could also use variance as a modal measure but this does a poor job at distinguishing distributions with a higher number of modes.

The modal phenomena is not unique to the one dimensional Hadamard walk and occurs in a variety of two dimensional absorbing walks as well. We display these in Figure 10.

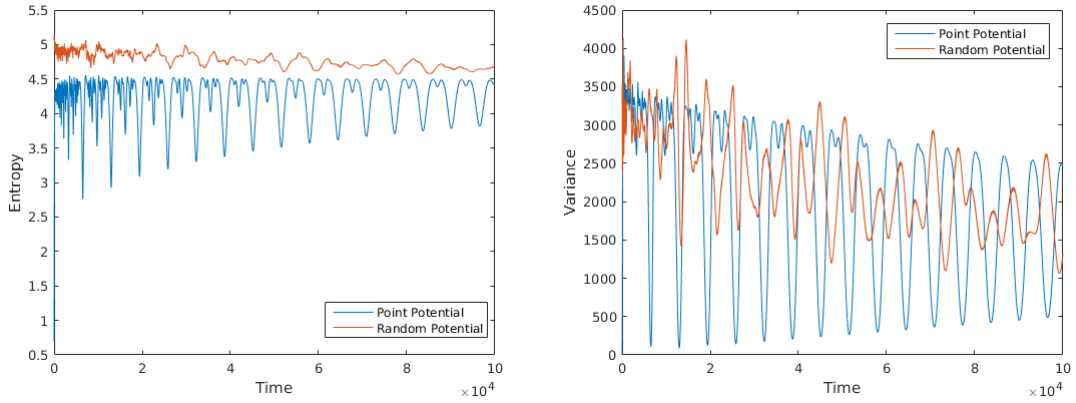


Figure 4.9: (*Left*) Plot of entropy over time for the $(\mathbb{Z}, C_1, H, \{0, n\})$ quantum walk (*Right*) Plot of variance over time for the $(\mathbb{Z}, C_1, H, \{0, n\})$ quantum walk

4.6 Conclusion

In this paper we have illustrated spectral differences between the classical random walk and different forms of the quantum walk for both periodic and absorbing boundary conditions. The eigenvalues of the absorbing walks approach that of the periodic walks, and the eigenvectors of the absorbing quantum walk approximate the squared eigenvectors of the classical random walk. The difficulties in computing exact spectra for the absorbing quantum walk can be traced back to the governing polynomial recursion of the characteristic polynomial. Furthermore, we introduced modal phenomena, or the periodic emergence of regularly spaced peaks in the conditional distribution of an absorbing quantum walk. The precise mechanism behind this phenomena and approximations of these modal distributions are still unknown, and a more complete analysis remains to be done.

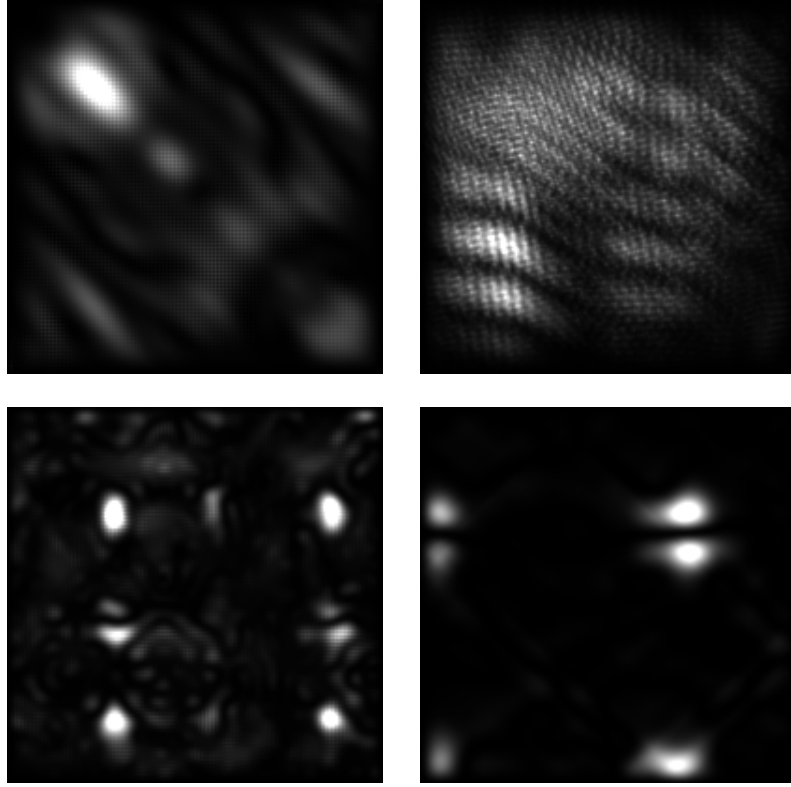


Figure 4.10: Illustrations of modal phenomena in a variety of two dimensional quantum walks (*Top Left*) Conditional distribution of the $(\mathbb{Z}^2, C_2, U(0.7) \otimes U(0.3), B_{X,Y})$ absorbing walk at time $t = 29300$ for $X = Y = 100$ and an initial position of $|(54, 54)\rangle$ (*Top Right*) Conditional distribution of the $(\mathbb{Z}^2, \Sigma, U(0.8) \otimes U(0.9) \otimes U(0.3), B_{X,Y})$ absorbing walk at time $t = 18130$ for $X = Y = 100$, $\Sigma = \{(1, 0), (-2, 2), (1, 4), (0, -2), (1, 5), (0, 4), (0, 1), (-2, 0)\}$, and an initial position of $|(52, 152)\rangle$ (*Bottom Left*) Conditional distribution of the $(\mathbb{Z}^2, \tilde{C}_2, G_5, B_{X,Y} \cup \{(x, y)\})$ absorbing walk at time $t = 28920$ for $X = Y = 100$ and an initial position of $|(x, y)\rangle = |(92, 84)\rangle$ (*Bottom Right*) Conditional distribution of the $(\mathbb{Z}^2, C_2, G_4, B_{X,Y} \cup \{(x, y)\})$ absorbing walk at time $t = 17230$ with $X = Y = 100$ and an initial position of $|(x, y)\rangle = |(9, 77)\rangle$

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