Quantum Walks and Pretty Good State Transfer on Paths

by

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I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

Quantum computing is believed to provide many advantages over traditional computing, particularly considering the speed at which computations can be performed. One of the challenges that needs to be resolved in order to construct a quantum computer is the transmission of information from one part of the computer to another. Quantum walks, the quantum analogues of classical random walks, provide one potential method for resolving this challenge.

In this thesis, we use techniques from algebraic graph theory and number theory to analyze the mathematical model for continuous time quantum walks on graphs. For the continuous time quantum walk model, we define a transition operator, which is a function of a Hamiltonian. We focus on the cases where the adjacency matrix or the Laplacian of a graph act as the Hamiltonian. We mainly consider quantum walks on paths as a model for spin chains, which are the underlying basis of a quantum communication protocol.

For communication to be efficient, we desire states to be transferred with high fidelity, a measure of the amount of similarity between the transmitted state and the received state. At the maximum fidelity of 1, we say we have achieved perfect state transfer. Examples of perfect state transfer are relatively rare, so the concept of pretty good state transfer was introduced as a natural relaxation, which exists if fidelities arbitrarily close to 1 are obtained.

Our first main result is to characterize pretty good state transfer on paths. Previously, pretty good state transfer on paths was considered mainly for the end vertices, though results for both models indicated that if there was pretty good state transfer between the end vertices, then there was pretty good state transfer between internal vertices equidistant from each end. We complete the characterization by demonstrating, for the adjacency matrix model, a family of paths where pretty good state transfer exists between internal vertices but not between end vertices, and verifying that no other example exists. For the Laplacian model, we show that there are no paths with pretty good state transfer between internal vertices but not between the end vertices.

Our second main result considers initial states involving multiple vertices. Under the adjacency matrix model, we provide necessary and sufficient conditions for pretty good state transfer in a particular family of paths in terms of the eigenvalue support of the initial state. We also discuss recent results on fractional revival, which is another form of multiple qubit state transfer.

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Dedication

To Jamie

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List of Symbols

*	complex conjugate
$\dagger$	conjugate transpose
$\square$	Cartesian product
$\otimes$	Kronecker product
$\sim$	denotes adjacency
$A(X)$	the adjacency matrix of a graph X
$\text{adj}(M)$	the adjoint matrix of M
$\mathsf{Aut}_X(a)$	the group of automorphisms of X that fix vertex a
$\mathbb{C}$	the set of complex numbers
C_n	the cycle on n vertices
$\Delta(X)$	the degree matrix of a graph X
$\det(M)$	the determinant of a matrix M
$E(X)$	the edge set of a graph X
E_λ	the orthogonal projection onto the eigenspace of λ
$\mathbf{e}_v$	the elementary vector corresponding to vertex v; contains a 1 in the row corresponding to v, and all other entries are 0
$\text{ev}(M)$	the set of eigenvalues of a matrix (or graph) M
I	the identity matrix
J	the all-ones matrix
K_n	the complete graph on n vertices
$K_{m,n}$	the complete bipartite graph with parts of size m and n
$L(X)$	the Laplacian of a graph X
$M(t)$	mixing matrix or probability matrix of a walk
$\mathbb{N}$	the set of positive integers
$N(a)$	the open neighbourhood of a vertex a
$N[a]$	the closed neighbourhood of a vertex a

P_n	the path on n vertices, typically with vertex set $V(P_n) = \{1, \ldots, n\}$ and edge set $E(P_n) = \{(j, j+1) : 1 \leq j < n\}$
$\Phi_m(x)$	the cyclotomic polynomial of order m
$\phi(M, x)$	the characteristic polynomial of a matrix (or graph) M in variable x
$\mathbb{Q}$	the set of rational numbers
$\mathbb{R}$	the set of real numbers
$S_{k,\ell}$	the double star graph formed by joining the non-leaf vertices of $K_{1,k}$ and $K_{1,\ell}$ by an edge
σ_r	the sign of $(E_r)_{a,b}$ or $\mathbf{w}^T E_r \mathbf{v}$ (where a, b or $\mathbf{v}, \mathbf{w}$ are understood from context)
sup	the supremum
^{T}	the transpose operator
Θ	the eigenvalue support, either of a vertex or a state
θ_j	the jth eigenvalue of a graph. For a path P_n, we let $\theta_j = 2\cos\left(\frac{\pi j}{n+1}\right)$
$U(t)$	the transition operator for a continuous time quantum walk
$V(X)$	the vertex set of a graph X
$\mathbf{v}$	arbitrary (multiple vertex) state, of the form $$\mathbf{v} = \sum_{x \in V(X)} \beta_x \mathbf{e}_x, \quad \sum_{x \in V(X)} \lvert\beta_x\rvert^2 = 1$$
$\mathbf{v}^\sigma$	the image of the state $\mathbf{v}$ under the automorphism σ, i.e. $$\mathbf{v}^\sigma = \sum_{x \in V(X)} \beta_x \mathbf{e}_{\sigma(x)}$$
$\mathbb{Z}$	the set of integers
$\mathbb{Z}_n$	the group of integers modulo n
ζ_j	$(1 - \sigma_j)/2$

Chapter 1

Introduction

Interest in quantum computing has grown steadily throughout the last number of years. The essence behind quantum computing is to take advantage of the laws of quantum mechanics to perform computations, for example, *superposition*, which is the ability of a quantum system to exist in multiple states simultaneously, and *entanglement*, which is a potential property of quantum particles that allow them to act as if they are linked, regardless of how far apart they are. These properties allow a quantum computer to perform many calculations simultaneously, allowing for solutions to problems to be obtained much faster.

A key requirement for the construction of a quantum computer is the ability to transmit information from one part of the computer to another. Because of the laws of quantum mechanics, and in particular the No-Cloning Theorem, information contained by a quantum particle cannot be copied, or at least, not without destroying the information contained by the original in the process. We focus here on the problem of *state transfer*: setting up a collection of qubits that allow this information to be transferred from one location to another, using *continuous time quantum walks*. Ideally, we would be able to achieve *perfect state transfer*, that is, starting from an initial state and allowing the walk to occur for a specified length of time, finding the same state at a different location. Because the precise set of conditions required to achieve this phenomenon are relatively rare, we relax this requirement and set as our goal *pretty good state transfer*, the ability to find a state arbitrarily close to the initial state at the desired location.

Our focus is to consider the mathematical model for continuous time quantum walks, and use techniques from algebraic graph theory and number theory to derive our results. To this end, we consider continuous time quantum walks as occurring on a graph, where the vertices model the qubits and the edges model the interactions between the qubits. Our primary goal is to provide a complete characterization of pretty good state transfer on paths and to begin to consider pretty good state transfer of multiple qubit states on paths. Some of the original contributions of this thesis are also contained in [21, 45].

Our secondary objective to to provide a detailed, self-contained overview of the theory used to investigate quantum walks and the developments that led to the investigation of pretty good state transfer on paths. We will first discuss the tools from graph theory, algebraic graph theory, and number theory used to study continuous time quantum walks. Then we will examine the properties of continuous time quantum walks and describe results for perfect and pretty good state transfer.

In this chapter, we provide an overview of the study of continuous time quantum walks and introduce our main results.

1.1 Model and Applications

Continuous time quantum walks were first investigated by Farhi and Gutmann [26] in 1998. They were considering decision problems, for example the travelling salesman problem and the exact cover problem, being modelled by a decision tree. By modelling a decision problem using a decision tree, determining the answer to the decision problem becomes equivalent to determining if there are any nodes at the nth level of the decision tree, for some parameter n. To solve the decision problem, the naïve approach is to systematically check every path starting from the top of the tree, attempting to find one that reaches the nth level. An alternative approach is to move through the tree according to a probabilistic rule, which includes a chance of back-tracking; eventually every node in the tree will be reached. More formally, a continuous time (classical) random walk is a Markov process. A family of trees is said to be *penetrable* if:

> There exists $A, B \geq 0$ such that for those trees with a node (or nodes) at the nth level there is a $t < n^A$ with the probability of being at the nth level by t greater than $(1/n)^B$.

Otherwise, the family of trees is said to be *impenetrable*.

Formally, given a graph X, we can define a *continuous random walk* on X by a family of matrices $M(t)$, where $M(t)_{a,b}$ denotes the probability that a "walker" starting on vertex a is found at vertex b after time t. The matrices $M(t)$ are given by

$$M(t) := \exp(t(A - \Delta)),$$

where A is the adjacency matrix of the graph and Δ is the degree matrix of the graph. The continuous random walk is modelled such that in a short time interval δt, the walker leaves the current vertex and moves to one of the adjacent vertices with equal probability. One thing worth noting here is that if the graph X is connected, then the matrix $M(t)$ will converge to a limiting distribution.

Farhi and Gutmann [26] investigated using quantum mechanics to move through decision trees, modelled by a continuous time quantum walk. We consider a continuous time quantum walk as a generalization of a continuous random walk. So analogously, we can define a *continuous time quantum walk* by defining a transition operator $U(t)$ in terms of a real symmetric matrix S, called the *Hamiltonian* of the walk, by

$$U(t) := \exp(itS) = \sum_{n\geq 0} \frac{(it)^n}{n!} S^n.$$

Comparing to the continuous random walk, the main difference in the set up is the introduction of the complex term i in the exponent, and the freedom to choose other possible models by varying S compared to the specific example for the continuous random walk. For a graph X, the most common choices for S are the adjacency matrix A and the Laplacian L. The model determined by A is often said to be determined by the XY-Hamiltonian, and the model determined by L is often said to be determined by the XYZ-Hamiltonian or Heisenberg Hamiltonian.

Farhi and Gutmann [26] set up a continuous time quantum walk using the Laplacian as the Hamiltonian, and defined *quantum penetrable* and *quantum impenetrable* analogously. They determined that any family of trees that is (classically) penetrable is also quantum penetrable. Moreover, they gave an example of a family of decision trees that is (classically) impenetrable but quantum penetrable, based on adding two infinite paths to a decision tree. In 2002, Childs, Farhi, and Gutmann [14] studied the difference in behaviour of a classical random walk and quantum walk and provided the family of finite graphs G_n, defined to be two balanced binary trees of depth n with the nth level vertices pairwise identified, which are (classically) impenetrable but quantum penetrable. In 2003, Childs et al. [13] remarked that this search problem can be solved in polynomial time by a classical algorithm, and modified the graph by joining the two sets of leaves by a cycle to construct a family of graphs that is quantum penetrable but which no classical algorithm can solve with high probability in subexponential time.

In 2004, Childs and Goldstone [16] considered the spatial search problem, where the algorithms are applied to a physical database as opposed to the idealized situation of calling an oracle, though the use of continuous time quantum walks. The use of quantum walks is natural to study this problem, as a graph can be used to model the locations and connections of the physical database. Their approach modifies the Hamiltonian used by introducing an oracle Hamiltonian, which is assumed to be given and indicates which state is goal of the search. They also use a uniform superposition as their starting state, in contrast to the work described previously which begins from a state representing a single vertex. The authors demonstrated their proposed walk matches the algorithm proposed for the complete graph by Farhi and Gutmann [25], and consider the results of their algorithm on the hypercube and the d-dimensional cubic periodic lattice. They were able to demonstrate quadratic speedups in dimensions greater than four, some speedup at dimension four, and no substantial speedup in lower dimensions. In a subsequent 2004 paper, Childs and Goldstone [15] demonstrated that by making use of additional memory, they can obtain quadratic speedup in dimensions greater than two, and some speedup at dimension two.

In 2002, Moore and Russell [39] studied quantum walks and uniform mixing, the question of whether the process reaches a uniform state (up to phase), on the hypercube. They determined that the n-dimensional hypercube has an instantaneous mixing time at $(\pi/4)n$, compared to a $\Theta(n \log n)$ mixing time in the classical case. Similarly, they define an *average mixing time*, analogous to the definition provided by Aharonov, Ambainis, Kempe, and Vazirani [1] in the discrete case, as a time at which the average distribution is uniform. For the hypercube, the limiting distribution is not the uniform distribution, and there is no average mixing time.

In 2003, Ahmadi, Belk, Tamon, and Wendler [2] further investigated instantaneous uniform mixing on graphs. One of their results is that on the class of complete and complete multipartite graphs, only the complete graphs K_2, K_3, K_4 and the compete multipartite graph $K_{2,2}$ have instantaneous uniform mixing, in stark contrast to the results for the classical walk, which never achieves uniform on K_2 but converges to uniform on K_n for all $n \geq 2$, and the discrete quantum walk. Moreover, K_2 is the only complete graph with average uniform mixing. The authors conjecture that no cycle on more than four vertices has instantaneous uniform mixing, and no Cayley graph on the symmetric group S_n with edges as transpositions with $n \geq 3$ has instantaneous uniform mixing. Later that year, Gerhardt and Watrous [28] demonstrated that Cayley graphs on the symmetric group S_n do not have instantaneous uniform mixing when the edges are generated by all p-cycles, for some fixed $2 \leq p \leq n$; the case $p = 2$ answers the latter question of Ahmadi, Belk, Tamon, and Wendler [2]. Additionally, Ahmadi, Belk, Tamon, and Wendler [2] appear to be the first to comment on the distinction between using the Laplacian and the adjacency matrix as the Hamiltonian, which on regular graphs simply introduces an irrelevant phase factor.

Also in 2003, Bose [6] developed the use of continuous time quantum walks to transmit quantum states between two locations. Transmission of quantum states is important to link quantum processes to allow for quantum computing on a larger scale. The two main methods of transferring quantum states are by doing so directly through such a transmission channel, or by sharing an entangled state through the transmission channel and later transferring the state by quantum teleportation. The model proposed is a spin chain, or in graph theoretic terms, a path, and transmission occurs by initializing the state at one end and waiting a predetermined amount of time for the state to naturally propagate to the other end. Such a model has the advantage of not requiring external inputs, such as turning interactions between parts of the chain on and off, or modulation from an outside source. These advantages make the model an ideal connector between quantum computers.

One of the major goals of quantum communication on spin chains is to transfer a state with high *fidelity*, a measure of the amount of similarity between the transmitted state and the received state. At the maximum fidelity of 1, the two states are the same (up to the phase factor, which cannot be determined by measurement), and we say we have achieved *perfect state transfer*. Formally, a graph X is said to have *perfect state transfer* between vertices a and b if there exist a time $\tau \in \mathbb{R}$ and a complex scalar γ such that

$$U(\tau)\mathbf{e}_a = \gamma \mathbf{e}_b,$$

where $\mathbf{e}_v$ denotes the vector with a 1 in the row corresponding to vertex v and with all other entries 0. Bose numerically studied the fidelity of the state transfer and preservation of entanglement across paths and cycles (at opposite points), and determined that C_4 allows transfer with a fidelity of 1. The concept of perfect state transfer was introduced by Christandl et al. [17, 18] in 2005, who also showed that perfect state transfer on uniformly coupled spin chains (or in graph theoretic terms, unweighted paths) is only possible for chains of two or three qubits. We provide a detailed overview of results for perfect state transfer in Chapter 3.

In 2009, Childs [12] determined that continuous time quantum walks are universal for quantum computation; that is, any problem that can be solved by a quantum computer can be solved using a quantum walk. More precisely, quantum gates and quantum circuits can be simulated by simple quantum walks on sparse graphs (unweighted graphs of bounded degree), and as it turns out, the same is true in reverse (see [13]). The model presented uses unweighted graphs with maximum degree 3. This result demonstrates the power of the continuous time quantum walk model and motivates developing further understanding of the model.

The lack of examples of perfect state transfer led multiple authors (see Godsil [32], for example) to introduce the concept of *pretty good state transfer* as a natural relaxation.

We discuss previous results for pretty good state transfer on paths in Section 4.2. In the following sections, we outline the main original contributions of this thesis.

1.2 Pretty Good State Transfer on Paths

Formally, a graph X is said to have *pretty good state transfer* between vertices a and b if, there exist sequences of times $\{\tau_k\}$ of real numbers and $\{\gamma_k\}$ of complex numbers with $|\gamma_k| = 1$, such that

$$\lim_{k\to\infty} \|U(\tau_k)\mathbf{e}_a - \gamma_k \mathbf{e}_b\| = 0,$$

or equivalently, for every $\epsilon > 0$, there exist $\tau_\epsilon \in \mathbb{R}$ and $\gamma_\epsilon \in \mathbb{C}$ with $|\gamma_\epsilon| = 1$, such that

$$\|U(\tau_\epsilon)\mathbf{e}_a - \gamma_\epsilon \mathbf{e}_b\| < \epsilon.$$

One of our main results is to complete the characterization of pretty good state transfer on paths, which was previously only considered between the end vertices of the path. We let P_n denote a path on n vertices, and assume the vertices are labelled 1 to n such that vertices with successive labels are adjacent. Godsil et al. [34] provided a characterization of pretty good state transfer between the end vertices of paths with the adjacency matrix as the Hamiltonian, showing pretty good state transfer occurs between the end vertices if and only if the length of the path is one less than either a prime, twice a prime, or a power of two. Banchi et al. [4] provided the analogous characterization with the Laplacian as the Hamiltonian, demonstrating pretty good state transfer occurs between the end vertices if and only if the length of the path is a power of two. In both cases, the authors commented that if there is pretty good state transfer between the end vertices of P_n (i.e. vertices 1 and n), then there is also pretty good state transfer between vertices a and $n+1-a$, but did not consider whether there could be pretty good state transfer between internal vertices of paths if it was not present between the end vertices. We will present the following results to complete these characterizations.

4.3.3 Theorem. *There is pretty good state transfer on P_n between vertices a and b if and only if $a + b = n + 1$ and:*

a) $n = 2^t - 1$, where t is a positive integer;

b) $n = p - 1$, where p is an odd prime; or

c) $n = 2^t p - 1$, where t is a positive integer and p is an odd prime, and a is a multiple of 2^{t-1}.

4.4.3 Theorem. *There is pretty good state transfer on P_n between vertices a and b with respect to the Laplacian if and only if $a + b = n + 1$ and n is a power of 2.*

1.3 State Transfer of Multiple Qubit States

Having completed the characterization of pretty good state transfer on paths with respect to an initial state involving a single qubit, or vertex, we will begin to analyze state transfer of arbitrary states involving multiple qubits (vertices), restricted to the single excitation case, that is, a state in the span of the elementary vectors. Hence, we define an initial state $\mathbf{v}$ of a graph X by

$$\mathbf{v} := \sum_{x \in V(X)} \beta_x \mathbf{e}_x, \qquad \sum_{x \in V(X)} |\beta_x|^2 = 1.$$

To generalize the concept of symmetry exhibited by a path, which motivates our desired output, a graph X has an *automorphism* σ if σ is a permutation of $V(X)$ such that vertices a and b are adjacent if and only if vertices $\sigma(a)$ and $\sigma(b)$ are adjacent. Then we define $\mathbf{v}^\sigma$ by

$$\mathbf{v}^\sigma := \sum_{x \in V(X)} \beta_x \mathbf{e}_{\sigma(x)}.$$

Formally, we say a graph X with automorphism σ has *perfect state transfer* between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if there exist a time $\tau \in \mathbb{R}$ and a complex scalar γ such that

$$U(\tau)\mathbf{v} = \gamma \mathbf{v}^\sigma,$$

and X has *pretty good state transfer* between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if there exist a sequences $\{\tau_k\}$ of real numbers and complex scalars $\{\gamma_k\}$ such that

$$\lim_{k \to \infty} \|U(\tau_k)\mathbf{v} - \gamma_k \mathbf{v}^\sigma\| = 0,$$

or equivalently, for every $\epsilon > 0$, there exists $\tau \in \mathbb{R}$ and $\gamma \in \mathbb{C}$ with $|\gamma| = 1$, such that

$$\|U(\tau)\mathbf{v} - \gamma \mathbf{v}^\sigma\| < \epsilon.$$

Our main result in this area is to identify examples of when pretty good state transfer of states can occur on paths. Sousa and Omar [43] demonstrated that with respect to the adjacency matrix, there is pretty good state transfer of any state on a path when the length of the path is one less than either a prime, twice a prime, or a power of two. It is a straightforward observation that there is pretty good state transfer in X between a state $\mathbf{v}$ and $\mathbf{v}^\sigma$ if there is pretty good state transfer between x and $\sigma(x)$ for every $x \in V(X)$ such that $\beta_x \neq 0$. For a path we will assume, without stating it explicitly, that the automorphism in question is that which takes vertex a to vertex $n+1-a$.

Our main results are for the class of *parity states*, a subset of the single-excitation states of paths which we define as follows. If $\mathbf{v}$ is such that $\beta_y = 0$ for all even y, we say that $\mathbf{v}$ is an *odd state*, and if $\mathbf{v}$ is such that $\beta_y = 0$ for all odd y, we say that $\mathbf{v}$ is an *even state*. Moreover, we say a state is a *parity state* if it is an odd state or an even state.

The following results are in terms of the *eigenvalues* of the path; more precisely, the *eigenvalue support* of the state. For a matrix S, we say that λ is an eigenvalue if there exists a nonzero vector w such that $Sw = \lambda w$; we call w an *eigenvector* with eigenvalue λ. The eigenvalues of P_n with respect to the adjacency matrix are given by

$$\theta_j := 2\cos\left(\frac{\pi j}{n+1}\right), \quad 1 \leq j \leq n.$$

The eigenvalue support of a state $\mathbf{v}$, denoted $\Theta_{\mathbf{v}}$, is the set of eigenvalues λ such that if E_λ is the orthogonal projection onto the eigenspace of λ, then $E_\lambda \mathbf{v} \neq \mathbf{0}$.

5.1.10 Theorem. *Suppose $m = 2^t p^s$, where p is an odd prime and $s, t > 0$, and let $\mathbf{v}$ be a parity state of P_{m-1}. For $1 \leq c < m/p$, let*

$$S_c := \{\theta_{c+jm/p} : 0 \leq j < p\}.$$

Moreover, let $S_0 := \{\theta_{m/2}\}$ be given. Then in P_{m-1}, there is pretty good state transfer between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if and only if there does not exist S_c with c odd and $S_{c'}$ with c' even such that $S_c \cup S_{c'} \subseteq \Theta_{\mathbf{v}}$.

5.1.11 Theorem. *Suppose $m = p^s$, where p is an odd prime and $s > 0$, and let $\mathbf{v}$ be a parity state of P_{m-1}. For $1 \leq c < m/(2p)$, let*

$$R_c := \{\theta_{c+jm/p} : 0 \leq j < p\} \cup \{\theta_{m/p-c+jm/p} : 0 \leq j < p\}.$$

Then in P_{m-1}, there is pretty good state transfer between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if and only if there does not exist R_c such that $R_c \subseteq \Theta_{\mathbf{v}}$.

Chapter 2

Algebra, Graphs, and Number Theory

In this chapter, we provide an overview of the basic definitions and theory from algebraic graph theory and number theory that will be used throughout this work. For more details, or additional background, we refer the reader to Godsil and Royle [35] and Levitan and Zhikov [38], respectively. For further reading on quantum information and computation, we refer the reader to Nielsen and Chaung [40].

2.1 Graphs and Matrices

Throughout this work, we adopt the convention that I represents the identity matrix and J represents the all-ones matrix, each of the appropriate order for the calculation to make sense.

A *graph* X is determined by a set of vertices $V(X)$ and a set of edges $E(X)$, where each edge is a 2-element subset of $V(X)$. If $\{a, b\}$ is an edge of the graph X, we will usually use ab as a shorthand notation for the edge, and we say that a and b are adjacent or that a is a neighbour of b, and denote this concept using $a \sim b$. A vertex is *incident* with an edge if it is one of the two vertices that forms the edge. We will assume a graph is both *simple*, that is, that there is at most one edge between each set of vertices, and every edge is undirected, and finite, i.e., $|V(X)|$ is finite, unless stated otherwise.

A *complete graph* is a graph in which every pair of vertices is adjacent. We denote the complete graph on n vertices by K_n. A *complete bipartite graph* is a graph in which the set of vertices is partitioned into two sets, and two vertices are adjacent if and only if they are in different sets of the partition. We denote the complete bipartite graph with sets of vertices of size m and n by $K_{m,n}$. A *cycle* on n vertices is a graph in which the vertices are connected in a single closed chain. We denote the cycle on n vertices by C_n. A *path* on n vertices is a graph such that there exists an ordering of the vertex set $a_1, a_2, \ldots, a_n$ such that the edge set is given by $\{\{a_i, a_{i+1}\}, 1 \leq i < n\}$. We denote the path on n vertices by P_n. Unless otherwise stated, we will assume $V(P_n) = \{1, 2, \ldots, n\}$ and $E(P_n) = \{\{1, 2\}, \{2, 3\}, \ldots, \{n-1, n\}\}$.

The *adjacency matrix* of a graph X, denoted $A(X)$, is the matrix with rows and columns indexed by the vertices of X, such that the (a, b)-entry of $A(X)$ is equal to 1 if a and b are adjacent, and 0 otherwise. By definition, $A(X)$ is symmetric. The *degree matrix* of X, denoted $\Delta(X)$, is the diagonal matrix of the degrees of the vertices of X. The *Laplacian* of X, denoted $L(X)$, is given by $\Delta(X) - A(X)$. We observe that for a given graph, none of these matrices are unique, as they depend on the order in which the vertices index the rows and columns. However, for most practical purposes, the order or labels of the vertices are not relevant to considering the properties of a graph. Hence, we say that two graphs are *isomorphic* if there is a bijection φ from $V(X)$ to $V(Y)$ such that $a \sim b$ in X if and only if $\varphi(a) \sim \varphi(b)$ in Y. We then call φ an *isomorphism* from X to Y. An *automorphism* is an isomorphism of a graph onto itself. While isomorphic graphs can have different adjacency matrices, degree matrices, or Laplacians based on the ordering of the vertices in the matrix, we can demonstrate a similar equivalence property at the matrix level as follows, expanding the result in [35], where a *permutation matrix* is a square 01-matrix that has precisely one 1 in each row and each column.

2.1.1 Lemma. *Let X and Y be graphs on the same vertex set. If they are isomorphic, then there is a permutation matrix P such that $P^T \Delta(X) P = \Delta(Y)$. Moreover, the following are equivalent:*

a) X and Y are isomorphic;

b) There is a permutation matrix P such that $P^T A(X) P = A(Y)$; and

c) There is a permutation matrix P such that $P^T L(X) P = L(Y)$.

Proof. Suppose X and Y are isomorphic graphs on the same vertex set, i.e. we have $V(X) = V(Y) := V$. Then there exists a bijection $\varphi : V \to V$ such that (a, b) is an edge of X if and only if $(\varphi(a), \varphi(b))$ is an edge of Y. Let P be the matrix with rows and columns indexed by V such that the (a, b)-entry of P is 1 if $\varphi(a) = b$ and 0 otherwise.

Then it is clear that P is a permutation matrix. We show that $P^T M(X)P = M(Y)$, where $M \in \{A, \Delta, L\}$. Consider the (a, b)-entry of $M(X)$. By matrix multiplication, this entry is the $(\varphi(a), \varphi(b))$ entry of $P^T M(X)P$, but by definition of isomorphism, this entry is also the $(\varphi(a), \varphi(b))$ entry of $M(Y)$ as desired.

Now suppose there is a permutation matrix P such that $P^T A(X)P = A(Y)$. Let φ be the bijection such that $b = \varphi(a)$ if and only if the (a, b)-entry of P is 1. Now suppose (a, b) is an edge in X, then the (a, b)-entry of $A(X)$ is 1. Since $(\varphi(a), \varphi(b))$ has the same entry in $A(Y)$, we obtain that $(\varphi(a), \varphi(b))$ is a directed edge in Y, and conversely. Hence, it follows that φ is an isomorphism.

Finally, suppose there is a permutation matrix P such that $P^T L(X)P = L(Y)$. By definition of the Laplacian, we have $P^T \Delta(X)P - P^T A(X)P = \Delta(Y) - A(Y)$. Since $P^T \Delta(X)P$ and $\Delta(Y)$ are diagonal matrices, and $P^T A(X)P$ and $A(Y)$ have zero diagonals, it follows that $P^T A(X)P = A(Y)$, and it again follows that φ is an isomorphism. □

We observe that permutation matrices are *orthogonal*, i.e, their columns (or rows) are orthogonal unit vectors. Hence it follows that if P is a permutation matrix, then $P^{-1} = P^T$. Therefore, if two graphs are isomorphic, then their adjacency matrices are *similar matrices*. Given this similarity, it suffices to pick an ordering of the vertices, and refer to *the* adjacency matrix, degree matrix, or Laplacian to be the one which corresponds to this ordering.

The *characteristic polynomial* of a matrix M is the polynomial

$$\phi(M, x) = \det(xI - M),$$

and as a shorthand, we denote the characteristic polynomial of $A(X)$ by $\phi(X, x)$. The *spectrum* of a matrix is a list of its eigenvalues and their multiplicities; the spectrum of a graph is the spectrum of its adjacency matrix (and similarly many linear algebra concepts, such as eigenvalues and eigenvectors, are applied to graphs by applying them to their adjacency matrices). If X and Y are isomorphic, then $\phi(X, x) = \phi(Y, x)$, as demonstrated in the following corollary.

2.1.2 Corollary. *[35] Let X and Y be graphs. If X and Y are isomorphic, then*

$$\phi(X, x) = \phi(Y, x).$$

Proof. Since X and Y are isomorphic, then by Lemma 2.1.1, there exists a permutation matrix P such that $P^T A(X)P = A(Y)$. The characteristic polynomial of Y is given by

$$\phi(Y, x) = \det(xI - A(Y))$$

and so we obtain

$$\phi(Y, x) = \det(xI - P^T A(X) P).$$

Since $P^{-1} = P^T$, we can introduce the factor $I = P^T P$ to obtain

$$\phi(Y, x) = \det(P^T P x I P^T P - P^T A(X) P) = \det(P^T (P x P^T - A(X)) P).$$

Using the determinant properties that $\det(AB) = \det(A)\det(B)$ and $\det(A^{-1}) = \det(A)^{-1}$, we obtain

$$\phi(Y, x) = \det(P^T)\det(xI - A(X))\det(P) = \det(xI - A(x)) = \phi(X, x)$$

as desired. □

Hence, we have observed that the characteristic polynomial, and hence the spectrum, is an invariant of the isomorphism class of a graph. However, the converse does not hold, and the spectrum of a graph does not necessarily determine its isomorphism class, as demonstrated in the following example.

2.1.3 Example. Let us consider the graphs $X = K_{1,4}$ and $Y = K_1 \cup C_4$. We calculate the characteristic polynomials of these graphs and obtain

$$\begin{aligned}
\phi(X, x) &= \det(xI - A(X)) \\
&= \det \begin{pmatrix} x & -1 & -1 & -1 & -1 \\ -1 & x & 0 & 0 & 0 \\ -1 & 0 & x & 0 & 0 \\ -1 & 0 & 0 & x & 0 \\ -1 & 0 & 0 & 0 & x \end{pmatrix} \\
&= -\det \begin{pmatrix} -1 & -1 & -1 & -1 \\ x & 0 & 0 & 0 \\ 0 & x & 0 & 0 \\ 0 & 0 & x & 0 \end{pmatrix} + x \begin{pmatrix} x & -1 & -1 & -1 \\ -1 & x & 0 & 0 \\ -1 & 0 & x & 0 \\ -1 & 0 & 0 & x \end{pmatrix} \\
&= -\det \begin{pmatrix} x & 0 & 0 \\ 0 & x & 0 \\ 0 & 0 & x \end{pmatrix} + x \det \begin{pmatrix} -1 & -1 & -1 \\ x & 0 & 0 \\ 0 & x & 0 \end{pmatrix} + x^2 \det \begin{pmatrix} x & -1 & -1 \\ -1 & x & 0 \\ -1 & 0 & x \end{pmatrix} \\
&= -x^3 - x \det \begin{pmatrix} x & 0 \\ 0 & x \end{pmatrix} - x^2 \det \begin{pmatrix} -1 & -1 \\ x & 0 \end{pmatrix} + x^3 \det \begin{pmatrix} x & -1 \\ -1 & x \end{pmatrix}
\end{aligned}$$

$$= -x^3 - x^3 - x^3 + x^4 - x^3$$

$$= x^4 - 4x^3,$$

and

$$\begin{aligned}
\phi(Y,x) &= \det(xI - A(Y)) \\
&= \det \begin{pmatrix} x & 0 & 0 & 0 & 0 \\ 0 & x & 1 & 0 & 1 \\ 0 & 1 & x & 1 & 0 \\ 0 & 0 & 1 & x & 1 \\ 0 & 1 & 0 & 1 & x \end{pmatrix} \\
&= x \det \begin{pmatrix} x & 1 & 0 & 1 \\ 1 & x & 1 & 0 \\ 0 & 1 & x & 1 \\ 1 & 0 & 1 & x \end{pmatrix} \\
&= x^2 \det \begin{pmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{pmatrix} - x \det \begin{pmatrix} 1 & 1 & 0 \\ 0 & x & 1 \\ 1 & 1 & x \end{pmatrix} - x \det \begin{pmatrix} 1 & x & 1 \\ 0 & 1 & x \\ 1 & 0 & 1 \end{pmatrix} \\
&= x^3 \det \begin{pmatrix} x & 1 \\ 1 & x \end{pmatrix} - x^2 \det \begin{pmatrix} 1 & 1 \\ 0 & x \end{pmatrix} - x \det \begin{pmatrix} x & 1 \\ 1 & x \end{pmatrix} + x \det \begin{pmatrix} 0 & 1 \\ 1 & x \end{pmatrix} \\
&\quad - x \det \begin{pmatrix} x & 1 \\ 1 & x \end{pmatrix} - x \det \begin{pmatrix} 1 & x \\ 0 & 1 \end{pmatrix} \\
&= x^4 - x^3 - x^3 - x^3 + x - x - x^3 + x - x \\
&= x^4 - 4x^3.
\end{aligned}$$

Hence, we observe that the two graphs are not isomorphic (one is connected and the other is not), but have the same characteristic polynomial and the same spectrum. ♢

Two graphs with the same spectrum are said to be *cospectral*. We can observe from the previous example that the spectrum cannot determine if a graph is connected or the valencies of the vertices.

2.2 Spectral Decomposition

The main algebraic graph theory tool we will use in this thesis is the spectral decomposition of a graph, which will allow us to simplify calculations of functions of the matrices in our later work. The goal of this section will be to demonstrate the spectral theorem for *Hermitian matrices* on $\mathbb{C}^n$, that is, matrices H such that $H^\dagger = H$. (Most of the matrices we will be considering are real symmetric, but at times we will need the full generality.) As a consequence, we obtain the spectral decomposition of Hermitian matrices. We begin with a demonstration of the existence of an orthonormal basis of $\mathbb{C}^n$ consisting of eigenvectors of a Hermitian matrix; it is a natural extension of the presentation of Godsil and Royle [35] for real symmetric matrices.

2.2.1 Theorem (Spectral Theorem). *Let H be a Hermitian $n \times n$ matrix. Then $\mathbb{C}^n$ has an orthonormal basis consisting of eigenvectors of H. Moreover, each eigenvalue of H is real, and if H is real, each eigenvector of H in the orthonormal basis can be chosen to be real.*

Proof. We claim we can find a set of n orthonormal eigenvectors of H, which forms a basis of $\mathbb{C}^n$. We proceed by induction, and let S be a set of orthonormal eigenvectors of H. Suppose $|S| = k < n$, then we demonstrate a set of $k+1$ eigenvectors.

Let $S = \{v_1, v_2, \ldots, v_k\}$, let v_i have eigenvalue θ_i, and let U be the space of linear combinations of the vectors in S. If $u \in U$, we can write $u = \sum_{i=1}^k c_i v_i$ and obtain

$$Hu = H \sum_{i=1}^{k} c_i v_i = \sum_{i=1}^{k} c_i H v_i = \sum_{i=1}^{k} c_i \theta_i v_u,$$

so Hu is a linear combination of the vectors in S and hence is in U. Hence, we see that for all $u \in U$, $Hu \in U$. Consider the orthogonal subspace $U^\perp$. If $v \in U^\perp$ and $u \in U$, then

$$\langle Hv, u \rangle = \langle v, Hu \rangle = 0,$$

since $Hu \in U$. Hence, $Hv \in U^\perp$, so for all $v \in U^\perp$, we have $Hv \in U^\perp$.

We now find an eigenvector of H in $U^\perp$. Let R be a matrix whose columns form an orthonormal basis for $U^\perp$, then $R^\dagger R = I$. For every column r_i of R, we have that $Hr_i \in U^\perp$, so there exists a vector b such that $Hr_i = Rb_i$. So if B is the square matrix whose columns are the b_i's we obtain $HR = RB$, and further

$$R^\dagger H R = R^\dagger R B = B,$$

demonstrating that H and B are similar matrices, and hence B is Hermitian. By the Fundamental Theorem of Algebra, B has at least one eigenvalue λ with corresponding eigenvector x. We see that

$$HRx = RBx = \lambda Rx,$$

so Rx is an eigenvector of H in $U^\perp$; moreover $Rx \neq 0$ as $x \neq 0$ by definition and the columns of R are linearly independent. Hence, we take v_{k+1} to be the unit vector corresponding to Rx, and by construction $S \cup \{v_{k+1}\}$ is a set of $k+1$ orthonormal eigenvectors. It follows therefore by induction that $\mathbb{C}^n$ has an orthonormal basis consisting of eigenvectors of H.

Moreover, if λ is an eigenvalue of H with eigenvector v, then

$$\lambda\langle v, v\rangle = \langle Av, v\rangle = \langle v, Av\rangle = \bar{\lambda}\langle v, v\rangle,$$

from which it follows that $\lambda = \bar{\lambda}$, i.e. λ is real. If H is real, we consider $v = x + iy$, where $x, y \in \mathbb{R}^n$, and obtain

$$\lambda x + i\lambda y = \lambda v = Hv = H(x + iy) = Hx + iHy.$$

As at least one of x or y is nonzero, it follows that there is a real eigenvector with eigenvalue λ, completing the proof. □

Let $\mathrm{ev}(H)$ denote the set of eigenvalues of H and for each eigenvalue θ of H, let E_θ be the matrix representing the orthogonal projection onto the eigenspace of θ. The *spectral decomposition* of H can now be obtained.

2.2.2 Lemma. *For a Hermitian matrix H, we have*

$$H = \sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta$$

Proof. Suppose H is an $n \times n$ matrix and let x be an arbitrary vector in $\mathbb{C}^n$. By Theorem 2.2.1, $\mathbb{C}^n$ has an orthonormal basis $\{v_1, \dots, v_n\}$ consisting of eigenvalues of H, where θ_i is the eigenvalue of v_i. Then there exist $\{c_i\}_{i=1}^n$ such that $x = \sum_{i=1}^n c_i v_i$. Now we see

$$\sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta x = \sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta \left(\sum_{i=1}^n c_i v_i \right) = \sum_{i=1}^n c_i \sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta v_i.$$

We observe that if x and y are eigenvalues of H with (real) eigenvalues λ and μ respectively, and $\lambda \neq \mu$, then x and y are orthogonal since

$$\lambda\langle x, y\rangle = \langle \lambda x, y\rangle = \langle Hx, y\rangle = \langle x, Hy\rangle = \langle x, \mu y\rangle = \mu\langle x, y\rangle,$$

and as λ, μ are distinct, we have $\langle x, y \rangle = 0$ as desired. Hence we obtain

$$\sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta x = \sum_{i=1}^{n} c_i \theta_i v_i.$$

By definition, we have that $\theta_i v_i = H v_i$, which gives us

$$\sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta x = \sum_{i=1}^{n} c_i H v_i = H \sum_{i=1}^{n} c_i v_i = Hx.$$

Therefore, for all $x \in \mathbb{C}^n$, we have

$$\left(\sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta - H \right) x = 0,$$

which implies H and $\sum_{\theta \in \mathrm{ev}(H)} \theta E_\theta$ are equal, completing the proof. □

The following more general result follows similarly.

2.2.3 Corollary. *For a Hermitian matrix H, and any polynomial p, we have*

$$p(H) = \sum_{\theta \in \mathrm{ev}(H)} p(\theta) E_\theta.$$

We demonstrate this tool through the following example.

2.2.4 Example. Let's find the spectral decomposition of P_3. We first calculate its characteristic polynomial:

$$\begin{aligned}
\phi(P_3, x) &= \det(xI - A(P_3)) \\
&= \det \begin{pmatrix} x & 1 & 0 \\ 1 & x & 1 \\ 0 & 1 & x \end{pmatrix} \\
&= x \det \begin{pmatrix} x & 1 \\ 1 & x \end{pmatrix} - \det \begin{pmatrix} 1 & 1 \\ 0 & x \end{pmatrix} \\
&= x^3 - x - x \\
&= x(x^2 - 2)
\end{aligned}$$

Hence we see that the eigenvalues of P_3 are $\sqrt{2}$, 0, and $-\sqrt{2}$. We next find a normalized eigenvector associated with each eigenvalue as

$$\frac{1}{2}\begin{pmatrix}1\\ \sqrt{2}\\ 1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ 0\\ -1\end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix}1\\ -\sqrt{2}\\ 1\end{pmatrix}$$

and since the eigenvalues are simple, each idempotent is of the form zz^T, where z is a normalized eigenvector. So we obtain the spectral decomposition

$$\sqrt{2}\times\frac{1}{4}\begin{pmatrix}1 & \sqrt{2} & 1\\ \sqrt{2} & 2 & \sqrt{2}\\ 1 & \sqrt{2} & 1\end{pmatrix} + 0\times\frac{1}{2}\begin{pmatrix}1 & 0 & -1\\ 0 & 0 & 0\\ -1 & 0 & 1\end{pmatrix} + -\sqrt{2}\times\frac{1}{4}\begin{pmatrix}1 & -\sqrt{2} & 1\\ -\sqrt{2} & 2 & -\sqrt{2}\\ 1 & -\sqrt{2} & 1\end{pmatrix}. \quad \diamond$$

2.3 Strongly Cospectral Vertices

In our investigation of quantum walks, the concept of strongly cospectral vertices will be a key factor in several results. Our treatment follows the work of Godsil and Smith [36]. We begin this section with the definition of cospectral vertices, first introduced by Schwenk [42]. Given a graph X, two vertices a and b are *cospectral* if $\phi(X\setminus a, x) = \phi(X\setminus b, x)$; i.e. the graphs $X\setminus\{a\}$ and $X\setminus\{b\}$ are cospectral. We introduce the following lemma to derive further properties of cospectral vertices; the result can be found in [29].

2.3.1 Lemma. *[29] Let X be a graph, v a vertex of X, and $\sum_\theta \theta E_\theta$ be the spectral decomposition of X. Then we have*

$$\frac{\phi(X\setminus v, x)}{\phi(X, x)} = \sum_\theta \frac{(E_\theta)_{v,v}}{x-\theta}.$$

Proof. Consider the expression $(xI - A(X))^{-1}$. Using spectral decomposition, we obtain

$$(xI - A(X))^{-1} = \sum_\theta \frac{1}{x-\theta}E_\theta.$$

On the other hand, using Cramer's rule, we obtain

$$(xI - A(X))^{-1} = \frac{\operatorname{adj}(xI - A(X))}{\det(xI - A(X))}.$$

So, looking at the (v, v) entry of $(xI - A(X))^{-1}$ and putting these two facts together, we obtain

$$\frac{\phi(X \setminus v, x)}{\phi(X, x)} = \frac{\mathrm{adj}(xI - A(X))_{v,v}}{\det(xI - A(X))} = (xI - A(X))^{-1}_{v,v} = \sum_{\theta} \frac{1}{x - \theta}(E_\theta)_{v,v},$$

as desired. □

We now provide an equivalent definition of cospectral vertices through the following lemma; additional characterizations can be found in [36, Theorem 3.1].

2.3.2 Lemma. *[36] Let a and b be vertices in X. Then a and b are cospectral if and only if for each idempotent E_θ in the spectral decomposition of X, we have $(E_\theta)_{a,a} = (E_\theta)_{b,b}$.*

Proof. Since a and b are cospectral, we have that $\phi(X \setminus a, x) = \phi(X \setminus b, x)$. It follows from the previous lemma that

$$\sum_{\theta} \frac{1}{x - \theta}(E_\theta)_{a,a} = \frac{\phi(X \setminus a, x)}{\phi(X, x)} = \frac{\phi(X \setminus b, x)}{\phi(X, x)} = \sum_{\theta} \frac{1}{x - \theta}(E_\theta)_{b,b},$$

from which it is clear that $(E_\theta)_{a,a} = (E_\theta)_{b,b}$, and conversely. □

As we will observe through the following lemma, it makes sense that strongly cospectral vertices are cospectral. The additional property that strongly cospectral vertices have that we will verify is that they are parallel. Two vertices a and b are *parallel* if for each eigenvalue θ, the vectors $E_\theta \mathbf{e}_a$ and $E_\theta \mathbf{e}_b$ are parallel, that is, there exists a constant c such that $E_\theta \mathbf{e}_a = cE_\theta \mathbf{e}_b$. Finally, we say that two vertices a and b are *strongly cospectral* if for each eigenvalue θ, we have $E_\theta \mathbf{e}_a = \pm E_\theta \mathbf{e}_b$.

2.3.3 Lemma. *[36] Two vertices a and b in X are strongly cospectral if and only if they are parallel and cospectral.*

Proof. Suppose a and b are strongly cospectral. It immediately follows from the definition that a and b are parallel. We verify that a and b are cospectral by observing

$$(E_r)_{a,a} = (E_r \mathbf{e}_a)_a = \pm(E_r \mathbf{e}_b)_a = \pm(E_r)_{a,b} = \pm(E_r)_{b,a} = \pm(E_r \mathbf{e}_a)_b = (E_r \mathbf{e}_b)_b = (E_r)_{b,b},$$

using the fact that the idempotents are symmetric.

Conversely, suppose a and b are parallel and cospectral. It follows that

$$\begin{aligned}(E_r)_{a,b} = (E_r)_{b,a} = (E_r\mathbf{e}_a)_b = c(E_r\mathbf{e}_b)_b = c(E_r)_{b,b} = c(E_r)_{a,a} = c(E_r\mathbf{e}_a)_a \\ = c^2(E_r\mathbf{e}_b)_a = c^2(E_r)_{a,b}\end{aligned}$$

again using the fact that idempotents are symmetric. Hence it follows that if $(E_r)_{a,b}$ is nonzero, then $c^2 = 1$, so $c = \pm 1$ as required.

Now consider the situation when $(E_r)_{a,b} = 0$. Since a and b are parallel, it follows that $(E_r)_{a,a} = (E_r)_{b,b} = 0$. We then observe that

$$||E_r\mathbf{e}_a||^2 = \mathbf{e}_a^T E_r^T E_r \mathbf{e}_a = \mathbf{e}_a^T E_r \mathbf{e}_a = (E_r)_{a,a} = 0,$$

using the fact that E_r is symmetric and idempotent. Similarly, $||E_r\mathbf{e}_b||^2 = 0$. Hence $E_r\mathbf{e}_a = E_r\mathbf{e}_b = 0$ as required. □

2.4 Eigenvalue Support and Covering Radius

An important consideration in our work in using the spectral decomposition is that not all the eigenvalues affect the calculations at a particular vertex. To this end, we introduce the notion of the eigenvalue support of a vertex. The results of this section largely follow the work of Coutinho and Godsil [20] and Godsil [31].

For a graph X, the *eigenvalue support* of a vertex a is the set of eigenvalues θ such that $E_\theta\mathbf{e}_a \neq 0$, and is denoted by Θ_a. Equivalently, Θ_a is the set of eigenvalues θ such that $(E_\theta)_{a,a} \neq 0$ since

$$(E_\theta)_{a,a} = \mathbf{e}_a^T E_\theta \mathbf{e}_a = \mathbf{e}_a^T E_\theta^2 \mathbf{e}_a = \mathbf{e}_a^T E_\theta^T E_\theta \mathbf{e}_a = ||E_\theta\mathbf{e}_a||^2.$$

We consider the following facts regarding the eigenvalue support. We begin with the result that the eigenvalues in the eigenvalue support of a vertex are the poles of the quotient of the characteristic polynomial of the subgraph not containing the vertex and the characteristic polynomial.

2.4.1 Lemma. *[20] The eigenvalue support of a vertex a in X consists of the eigenvalues θ such that θ is a pole of the rational function $\phi(X \setminus a, x)/\phi(X, x)$.*

Proof. By Lemma 2.3.1, we have

$$\frac{\phi(X \setminus a, x)}{\phi(X, x)} = \sum_\theta \frac{(E_\theta)_{a,a}}{x - \theta}.$$

It follows that θ is a pole of the LHS if and only if $(E_\theta)_{a,a} \neq 0$. □

Two complex numbers are said to be *algebraic conjugates* if they are roots of the same irreducible monic (minimal) polynomial with integer coefficients. It follows almost immediately that if an eigenvalue is in the eigenvalue support of a vertex, then so are its algebraic conjugates.

2.4.2 Corollary. *[20] If θ belongs to Θ_a, then so do all algebraic conjugates of θ.*

Proof. If θ is a root of $\phi(X, x)$ with greater multiplicity than of $\phi(X \setminus a, x)$, then a greater power of the minimal polynomial of θ divides $\phi(X, x)$ than $\phi(X \setminus a, x)$. The result follows. □

We conclude this section by considering a bound on the size of the eigenvalue support in terms of the following property of a graph. For a graph X, the *covering radius* of a vertex a is the smallest integer r such that for every $b \in V(X)$, the distance between a and b is at most r; this terminology is borrowed from coding theory. The following bound is obtained.

2.4.3 Lemma. *[31] For a graph X, if r is the covering radius of a, then $r < |\Theta_a|$.*

Proof. With respect to the adjacency matrix, the vectors $v_k := (A + I)^k \mathbf{e}_a$, for $0 \leq k \leq r$, are linearly independent as the size of the support of the vectors increases as k increases. Applying spectral decomposition, we obtain

$$v_k = (A + I)^k \mathbf{e}_a = \left(\sum_{\theta} (\theta + 1) E_\theta \right)^k \mathbf{e}_a = \sum_{\theta} (\theta + 1)^k E_\theta \mathbf{e}_a = \sum_{\theta \in \Theta_a} (\theta + 1)^k E_\theta \mathbf{e}_a.$$

Hence, there must be at least $r + 1$ eigenvalues in Θ_a.

With respect to the Laplacian, the vectors $v_k := (A + \Delta I)^k \mathbf{e}_a$, for $0 \leq k \leq r$, are linearly independent, and the result follows similarly. □

2.5 Almost Periodic Functions

To define almost periodic functions, we follow the treatment of Levitan and Zhikov [38]. Observe that a function f on $\mathbb{R}$ is *periodic* if there is a period τ such that for all t, we have that $f(t+\tau) = f(t)$. To generalize this notion to almost periodicity, we first generalize the notion of a period. We say that τ is an *ϵ-period* of a function f on $\mathbb{R}$ if for all t, we have that $|f(t+\tau) - f(t)| \leq \epsilon$. Then a function f on $\mathbb{R}$ is *almost periodic* if, for every $\epsilon > 0$, there exists an $\ell \in \mathbb{R}$ such that for every $t \in \mathbb{R}$, there exists a $\tau \in [t, t+\ell]$ such that τ is an ϵ-period of f. We call a subset T of $\mathbb{R}$ *relatively dense* if there is an $\ell > 0$ such that in every interval of length ℓ there is at least one element of T. Hence, we observe that an almost periodic function f has a relatively dense set $T(f, \epsilon)$ of ϵ-periods. We note that every periodic function is also almost periodic, and moreover the *trigonometric polynomial*

$$\sum_r a_r \exp(i\theta_r t),$$

with $a_r \in \mathbb{C}$ and $\theta_r \in \mathbb{R}$ is almost periodic. (Verifying that a sum of almost periodic functions is almost periodic is not trivial and we omit it here; for a proof, see for example [38, Property 1.6].)

Our later results will make extensive use of Kronecker's Theorem, which is stated and proved for completeness. In order to extend results on pretty good state transfer, the version we require is its more general strong form, which does not require the set of real numbers $\theta_0, \dots, \theta_d$ to be linearly independent over the rationals. Earlier works investigating state transfer have used a weaker version which does have this restriction, which we present as a corollary.

2.5.1 Theorem (Kronecker, see [38])**.** *Let $\theta_0, \dots, \theta_d$ and $\zeta_0, \dots, \zeta_d$ be arbitrary real numbers. For an arbitrarily small ϵ, the system of inequalities*

$$|\theta_r y - \zeta_r| < \epsilon \pmod{2\pi}, \quad (r = 0, \dots, d),$$

admits a solution for y if and only if, for integers $l_0, \dots, l_d$ such that

$$\ell_0\theta_0 + \cdots + \ell_d\theta_d = 0,$$

then

$$\ell_0\zeta_0 + \cdots + \ell_d\zeta_d \equiv 0 \pmod{2\pi}.$$

Proof. Suppose for every $\epsilon > 0$, there exists a y_ϵ such that

$$|\theta_r y_\epsilon - \zeta_r| < \epsilon \pmod{2\pi}, \quad (r = 0, \dots, d).$$

It follows there exist integers $m_0, \dots, m_d$ such that

$$-\epsilon < \theta_r y_\epsilon - \zeta_r - 2\pi m_r < \epsilon \qquad (r = 0, \dots, d).$$

Now suppose we have a set of integers $\ell_0, \ell_1, \ldots, \ell_d$ such that $\sum_{r=0}^{d} \ell_r \theta_r = 0$. Multiplying the inequality above by each ℓ_r and adding them together, we obtain

$$-\epsilon \sum_{r=0}^{d} |\ell_r| < y_\epsilon \sum_{r=0}^{d} \ell_r \theta_r - \sum_{r=0}^{d} \ell_r \zeta_r - 2\pi \sum_{r=0}^{d} \ell_r m_r < \epsilon \sum_{r=0}^{d} |\ell_r|,$$

and simplifying, we see that

$$\left| \sum_{r=0}^{d} \ell_r \zeta_r \right| < \epsilon \sum_{r=0}^{d} |\ell_r| \pmod{2\pi},$$

so since ϵ can be arbitrarily small, we must have that

$$\sum_{r=0}^{d} \ell_r \zeta_r \equiv 0 \pmod{2\pi},$$

as required.

Conversely, suppose for all sets of integers $\ell_0, \ldots, \ell_d$ such that

$$\ell_0 \theta_0 + \cdots + \ell_d \theta_d = 0,$$

we have that

$$\ell_0 \zeta_0 + \cdots + \ell_d \zeta_d \equiv 0 \pmod{2\pi}.$$

We begin by defining the following function

$$f(y) := 1 + \sum_{r=0}^{d} \exp[i(\theta_r y - \zeta_r)].$$

By applying the Triangle Inequality, we see that $|f(y)| \leq d + 2$:

$$|f(y)| \leq \left| 1 + \sum_{r=0}^{d} \exp[i(\theta_r y - \zeta_r)] \right| \leq 1 + \sum_{r=0}^{d} |\exp[i(\theta_r y - \zeta_r)]| \leq d + 2,$$

and observe that if $\sup |f(y)| = d + 2$, then for every $\epsilon > 0$, the system

$$|\theta_r y - \zeta_r| < \epsilon \pmod{2\pi}, \quad (r = 0, \ldots, d).$$

has a solution y_ϵ as follows. If $\sup |f(y)| = d + 2$, then for every $\delta > 0$, there exists a y_δ such that $|f(y_\delta)| > d + 2 - \delta$. Suppose for sake of contradiction that there exists an ϵ such that for every y there exists an s such that $|\theta_s y - \zeta_s| > \epsilon \pmod{2\pi}$. Note we may assume that $0 < \epsilon < \pi$. Setting $\delta = 2 - 2\cos(\epsilon/2)$, we obtain

$$\begin{aligned}
|f(y)| &= |1 + \sum_{r=0}^{d} \exp[i(\theta_r y - \zeta_r)]| \\
&\leq |1 + \exp[i(\theta_s y - \zeta_s)]| + \sum_{\substack{r=0 \\ r\neq s}}^{d} |\exp[i(\theta_s y - \zeta_s)]| \\
&\leq \sqrt{(1 + \exp[i(\theta_s y - \zeta_s)])(1 + \exp[-i(\theta_s y - \zeta_s)])} + d \\
&\leq 2|\cos[1/2(\theta_s y - \zeta_s)]| + d \\
&\leq 2|\cos[\epsilon/2]| + d \\
&\leq d + 2 - \epsilon,
\end{aligned}$$

contradicting that $\sup|f(y)| = d + 2$. Hence the system has a solution as desired.

We now demonstrate that $\sup|f(y)| = d + 2$. Define the function

$$F(x_0, x_1, \ldots, x_d) := 1 + x_0 + x_1 + \cdots + x_d.$$

Notice that when $x_k = \exp[i(\theta_k y - \zeta_k)]$, we have that $F(x_0, x_1, \ldots, x_d) = f(y)$. Observe that for n a positive integer, we have

$$F^n = \sum_{\substack{m_0, m_1, \ldots, m_d, m_{d+1} \\ m_0 + m_1 + \cdots + m_d + m_{d+1} = n}} \binom{n}{m_0\ m_1\ \cdots\ m_d\ m_{d+1}} x_0^{m_0} x_1^{m_1} \cdots x_d^{m_d},$$

$$f^n(y) = \sum_{\substack{m_0, m_1, \ldots, m_d, m_{d+1} \\ m_0 + m_1 + \cdots + m_d + m_{d+1} = n}} \binom{n}{m_0\ m_1\ \cdots\ m_d\ m_{d+1}} \prod_{k=0}^{d} \exp[m_k i(\theta_k y - \zeta_k)].$$

Now, let us simplify this expression into the form $f^n(y) = \sum_\nu \alpha_\nu \exp(i\beta_\nu t)$ by collecting terms. Then the coefficients are given by

$$\begin{aligned}
\alpha_\nu &= \sum_{\substack{m_0, m_1, \ldots, m_d, m_{d+1} \\ m_0 + m_1 + \cdots m_d + m_{d+1} = n \\ m_0\theta_0 + m_1\theta_1 + \cdots m_d\theta_d = \beta_\nu}} \binom{n}{m_0\ m_1\ \cdots\ m_d\ m_{d+1}} \prod_{k=0}^{d} \exp(-i m_k \zeta_k) \\
&= \sum_{\substack{m_0, m_1, \ldots, m_d, m_{d+1} \\ m_0 + m_1 + \cdots m_d + m_{d+1} = n \\ m_0\theta_0 + m_1\theta_1 + \cdots m_d\theta_d = \beta_\nu}} \binom{n}{m_0\ m_1\ \cdots\ m_d\ m_{d+1}} \exp(-i\gamma_\nu)
\end{aligned}$$

We now verify the above expression can be simplified as shown, i.e. that the expressions $m_0\zeta_0 + m_1\zeta_1 + \cdots m_d\zeta_d$ evaluate to a constant γ_ν. We see that

$$\begin{aligned} \beta_\nu = m_0\theta_0 + \cdots + m_d\theta_d = m_0'\theta_0 + \cdots + m_d'\theta_d \\ \implies (m_0 - m_0')\theta_0 + \cdots + (m_d - m_d')\theta_d = 0 \\ \implies (m_0 - m_0')\zeta_0 + \cdots + (m_d - m_d')\zeta_0 \equiv 0 \pmod{2\pi} \\ \implies m_0\zeta_0 + \cdots + m_d\zeta_d \equiv m_0'\zeta_0 + \cdots + m_d'\zeta_d \end{aligned}$$

as desired. Hence, we observe that

$$\sum_\nu |\alpha_\nu| = \sum_{\substack{m_0, m_1, \ldots, m_d, m_{d+1} \\ m_0 + m_1 + \cdots m_d + m_{d+1} = n \\ m_0\theta_0 + m_1\theta_1 + \cdots m_d\theta_d = \beta_\nu}} \binom{n}{m_0\ m_1\ \cdots\ m_d\ m_{d+1}} = (d+2)^n.$$

To complete the proof, we suppose for contradiction that $\sup|f(y)| = K < d+2$. Let

$$\mathcal{M}(f) := \lim_{T\to\infty} \frac{1}{T} \int_0^T f(y)dy.$$

We observe that $\mathcal{M}(f^n(y)\exp(-i\beta_\rho y)) = \alpha_\rho$:

$$\begin{aligned} \mathcal{M}(f^n(y)\exp(-i\beta_\nu y)) &= \mathcal{M}\left(\sum_\nu \alpha_\nu \exp(i\beta_\nu y)\exp(-i\beta_\rho y)\right) \\ &= \mathcal{M}\left(\alpha_\rho + \sum_{\nu\neq\rho} \alpha_\nu \exp(i(\beta_\nu - \beta_\rho)y)\right) \\ &= \mathcal{M}(\alpha_\rho) + \mathcal{M}\left(\sum_{\nu\neq\rho} \alpha_\nu \exp(i(\beta_\nu - \beta_\rho)y)\right) \\ &= \alpha_\rho, \end{aligned}$$

where the third inequality is given by the linearity of $\mathcal{M}(f)$ and the fourth is given by the periodicity of the complex exponential function.

Now we have

$$|\alpha_\rho| = |\mathcal{M}(f^n(y)\exp(-i\beta_\rho y))| \leq \mathcal{M}(|(f^n(y)\exp(-i\beta_\rho y)|) = \mathcal{M}(|f^n(y)|) \leq K^n.$$

Next, consider the number of terms in $F^n(x_0, x_1, \ldots, x_d)$. We claim it is at most $(n+1)^{d+1}$ terms. To see this, we proceed by induction on d. When $d = 0$, it is clear that the number of terms is at most $n+1$ as required. Now suppose for all n and a fixed $c \geq 0$, $F^n(x_0, x_1, \ldots, x_c)$ consists of at most $(n+1)^{c+1}$ terms. Then for $d = c+1$ we have

$$F^n(x_0, x_1, \ldots, x_c, x_{c+1}) = \sum_{m=0}^{n} \binom{n}{m} F^{n-m}(x_0, x_1, \ldots, x_c) x_{c+1}^m$$

and hence it is clear that the number of terms is bounded by $(n+1)(n+1)^{c+1} = (n+1)^{c+2}$, as desired.

Hence, we have

$$\sum_{\nu} |\alpha_\nu| \leq (n+1)^{d+1} K^n.$$

But then we see that

$$\lim_{n\to\infty} \frac{(n+1)^{d+1} K^n}{(d+2)^n} = \lim_{n\to\infty} (n+1)^{d+1} \left(\frac{K}{d+2}\right)^n = 0,$$

which demonstrates that the two expressions we have found for $\sum_\nu |\alpha_\nu|$ cannot simultaneously hold, which is the contradiction completing the proof. □

We note that the function $f(t)$ in the proof of Kronecker's Theorem is almost periodic, which implies that the set of solutions to the system of inequalities is relatively dense. In particular, there will be arbitrarily large solutions. We conclude this section by observing the following corollaries.

2.5.2 Corollary. *Let $\theta_0, \ldots, \theta_d$ be arbitrary real numbers. For an arbitrarily small ϵ, the system of inequalities*

$$|\theta_r y| < \epsilon \pmod{2\pi}, \quad (r = 0, \ldots, d)$$

admits a solution for y.

2.5.3 Corollary. *Let $\theta_0, \ldots, \theta_d$ be linearly independent real numbers over $\mathbb{Q}$, and $\zeta_0, \ldots, \zeta_d$ be arbitrary real numbers. For an arbitrarily small ϵ, the system of inequalities*

$$|\theta_r y - \zeta_r| < \epsilon \pmod{2\pi}, \quad (r = 0, \ldots, d),$$

admits a solution for y.

The latter result is also presented as a form of Kronecker's Theorem (see Bump [7]).

2.5.4 Theorem (Kronecker, as cited in [7])**.** *Let $(t_1, \ldots, t_r) \in \mathbb{R}^r$, and let t be the image of this point in $T = (\mathbb{R}/\mathbb{Z})^r$. Then t is a generator of T if and only if $1, t_1, \ldots, t_r$ are linearly independent over $\mathbb{Q}$.*

Chapter 3

Continuous Time Quantum Walks

We review the basic properties of continuous time quantum walks on graphs and then provide an overview of results for perfect state transfer and periodicity.

3.1 Properties

Recall that a *continuous time quantum walk* is defined by defining a transition operator $U(t)$ in terms of a real symmetric matrix S, commonly the adjacency matrix A or Laplacian L, called the *Hamiltonian* of the walk, by

$$U(t) := \exp(itS) = \sum_{n \geq 0} \frac{(it)^n}{n!} S^n.$$

Based on our discussion in Section 2.2, we observe we can also calculate the matrix $U(t)$ using the spectral decomposition of S to obtain

$$U(t) = \sum_{\theta \in \mathrm{ev}(S)} e^{it\theta} E_\theta.$$

Further, if we are interested in how the state evolves from starting at a particular vertex a, then we have

$$U(t)\mathbf{e}_a = \sum_{\theta \in \mathrm{ev}(S)} e^{it\theta} E_\theta \mathbf{e}_a,$$

and the only terms we need to consider are for the eigenvalues in the eigenvalue support of a.

Unlike the case of the continuous random walk (see Section 1.1), the transition matrix for the continuous quantum walk does not directly give the probability that a walker starting at a particular vertex is found at a given vertex. For that, we define the mixing matrix, denoted $M(t)$, to be the matrix obtained by taking as each entry the square of the absolute value of the corresponding entry of $U(t)$, or equivalently, we write

$$M(t) = U(t) \circ \overline{U(t)}$$

where $\overline{U(t)}$ is the matrix obtained from $U(t)$ by replacing every entry with its complex conjugate, and $\circ$ is the Schur product, or entry-wise product. Now $M(t)$ has the properties required to be a probability matrix. Notice that the entries of $M(t)$ are independent of the phase, or argument, of the value in $U(t)$, which reflects the fact that the phase of a quantum state is unable to be determined by measurement. We consider a continuous quantum walk for a small graph in the following example.

3.1.1 Example. Let us consider the example of a continuous quantum walk on K_2, the complete graph on two vertices, under both the adjacency matrix and the Laplacian models. For the adjacency matrix, we have

$$A = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

and since $A^{2k} = I$ and $A^{2k+1} = A$ for all $k \in \mathbb{Z}$, we have

$$\begin{aligned} U_A(t) &= \sum_{n \geq 0} \frac{(it)^n}{n!} A^n \\ &= \sum_{k \geq 0} \frac{(-1)^k (t)^{2k}}{(2k)!} I + \sum_{k \geq 0} \frac{i(-1)^k (t)^{2k+1}}{(2k+1)!} A \\ &= \cos(t) I + i \sin(t) A \\ &= \begin{pmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{pmatrix} \end{aligned}$$

and the resulting mixing matrix is

$$M_A(t) = \cos^2(t) I + \sin^2(t) A = \begin{pmatrix} \cos^2(t) & \sin^2(t) \\ \sin^2(t) & \cos^2(t) \end{pmatrix}.$$

For the Laplacian, we have

$$L = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

and since $L^k = 2^{k-1}L$ for all $k \in \mathbb{Z}^+$, we have

$$U_L(t) = \sum_{n\geq 0} \frac{(it)^n}{n!}L^n = \frac{1}{2}\left(J + \sum_{n\geq 0}\frac{(2it)^n}{n!}L\right) = \frac{1}{2}(J + e^{2it}L) = \frac{1}{2}\begin{pmatrix} 1+e^{2it} & 1-e^{2it} \\ 1-e^{2it} & 1+e^{2it}\end{pmatrix}$$

and the resulting mixing matrix is

$$M_L(t) = \frac{1}{2}(J + \cos(2t)L) = \frac{1}{2}\begin{pmatrix} 1+\cos(2t) & 1-\cos(2t) \\ 1-\cos(2t) & 1+\cos(2t)\end{pmatrix} = \begin{pmatrix} \cos^2(t) & \sin^2(t) \\ \sin^2(t) & \cos^2(t)\end{pmatrix}.$$

Let us now consider some extreme cases that occur on K_2. Consider the following scenarios:

$$M_A(\pi/4) = M_L(\pi/4) = \frac{1}{2}J$$

In this case, after time $\pi/4$, an initial state is mixed evenly between the vertices, and we say K_2 has *uniform mixing* at time $\pi/4$.

$$M_A(\pi/2) = M_L(\pi/2) = A$$

In this case, after time $\pi/2$, an initial state at a vertex is now found at the opposite vertex, and we say K_2 has *perfect state transfer* between its two vertices at time $\pi/2$.

$$M_A(\pi) = M_L(\pi) = I$$

In this case, after time π, the current state matches the initial state, and we say K_2 is periodic at time π. $\diamondsuit$

Formally, we say a graph X has *uniform mixing* if there exists a time $\tau \in \mathbb{R}$ such that $M(\tau) = |V(X)|^{-1}J$, or equivalently, if each entry of $U(\tau)$ has norm $|V(X)|^{-1}$. A graph X has *perfect state transfer* between vertices a and b if there exists a time $\tau \in \mathbb{R}$ such that $M(\tau)_{a,b} = 1$, or equivalently, if there exists a complex number γ with $|\gamma| = 1$ such that $U(\tau)\mathbf{e}_a = \gamma\mathbf{e}_b$. A graph X is *periodic* at a vertex a if there exists a time $\tau \in \mathbb{R}$ such that $M(\tau)_{a,a} = 1$, or equivalently, if there exists a complex number γ with $|\gamma| = 1$ such that $U(\tau)\mathbf{e}_a = \gamma\mathbf{e}_a$.

The times at which uniform mixing, perfect state transfer, and periodicity are achieved do not typically coincide under the two different models. In fact, a graph may have one of these properties under one model but not another. We observe this phenomenon in the following example.

3.1.2 Example. Let us consider the extreme cases that occur on P_3. The transition matrices for the two models are given by

$$U_A(\tau) = \frac{1}{4}e^{i\sqrt{2}\tau}\begin{pmatrix} 1 & \sqrt{2} & 1 \\ \sqrt{2} & 2 & \sqrt{2} \\ 1 & \sqrt{2} & 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix} + \frac{1}{4}e^{-i\sqrt{2}\tau}\begin{pmatrix} 1 & -\sqrt{2} & 1 \\ -\sqrt{2} & 2 & -\sqrt{2} \\ 1 & -\sqrt{2} & 1 \end{pmatrix},$$

$$U_L(\tau) = \frac{1}{3}\begin{pmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix} + \frac{1}{3}e^{3i\tau}\begin{pmatrix} 2 & -1 & -1 \\ -1 & 2 & -1 \\ -1 & -1 & 2 \end{pmatrix}.$$

Then we observe P_3 has perfect state transfer with respect to the adjacency matrix at time $\pi/\sqrt{2}$, but cannot have perfect state transfer with respect to the Laplacian. On the other hand, P_3 is periodic at time $\sqrt{2}\pi$ with respect to the adjacency matrix and time $2\pi/3$ with respect to the Laplacian. $\Diamond$

We further observe that taking Cartesian products of graphs preserves these properties. The *Cartesian product* of X and Y, denoted $X\square Y$, is the graph such that

$$V(X\square Y) = V(X) \times V(Y),$$
$$E(X\square Y) = \{(a,b)(c,d) : a = c \text{ and } bd \in E(Y) \text{ or } b = d \text{ and } ac \in E(X)\}.$$

The key tool that allows us to study the transition matrices of Cartesian product graphs is the Kronecker product. The *Kronecker product* of two matrices M and N, denoted $M \otimes N$, is the matrix we obtain by replacing the (i,j) entry of M by $M_{i,j}N$. Hence if M is a $k \times \ell$ matrix and N is an $m \times n$ matrix, then $M \otimes N$ is a $km \otimes \ell n$ matrix. An important property of Kronecker products is, if AC and BD are defined, then

$$(A \otimes B)(C \otimes D) = AC \otimes BD.$$

Using this property, we first provide a proof to verify the following identities (see [35], for example).

3.1.3 Proposition. *[35] Let X and Y be graphs, then*

a) $A(X\square Y) = A(X) \otimes I + I \otimes A(Y)$,

b) $\Delta(X\square Y) = \Delta(X) \otimes I + I \otimes \Delta(Y)$,

c) $L(X\square Y) = L(X) \otimes I + I \otimes L(Y)$.

Proof. a) Suppose the $((a,b),(c,d))$ entry of $A(X\Box Y)$ is 1. By definition, either $a=c$ and $bd \in E(Y)$ or $b=d$ and $ac \in E(X)$. In the former case, the $((a,b),(c,d))$ entry of $I\otimes A(Y)$ is 1 and the corresponding entry of $A(X)\otimes I$ is 0, and in the latter case, the $(a,b),(c,d)$ entry of $A(X)\otimes I$ is 1 and the corresponding entry of $I\otimes A(Y)$ is 0. Conversely, suppose the $((a,b),(c,d))$ entry of $A(X\Box Y)$ is 0. If $ac\in E(X)$, then $b\neq d$; if $bd\in E(Y)$, then $a\neq c$; otherwise $ac\notin E(X)$ and $bd\notin E(Y)$. In all three of these cases, the $((a,b),(c,d))$ entries of $A(X)\otimes I$ and $I\otimes A(Y)$ are zero.

b) It is clear that both expressions are diagonal matrices, so consider the $((a,b),(a,b))$ entries. The $((a,b),(a,b))$ entry of $\Delta(X)\otimes I$ is the degree of a in X, and the $((a,b),(a,b))$ entry of $I\otimes\Delta(Y)$ is the degree of b in Y. Since the degree of (a,b) in $X\Box Y$ is the sum of these two degrees by definition, the result follows.

c) Follows from the fact that $L(X)=\Delta(X)-A(X)$. □

Coutinho and Godsil demonstrated the following result relating the transition matrix of a Cartesian product to the transition matrices of the original graphs; the proof is reproduced for completeness.

3.1.4 Lemma. *[20] If X and Y are graphs, and $U(t)$ is defined in terms of A or L, then*

$$U_{X\Box Y}(t)=U_X\otimes U_Y$$

Proof. Let S represent the matrix defining $U(t)$. For all choices of S, the previous proposition gives us that $S(X\Box Y)=S(X)\otimes I+I\otimes S(Y)$. Moreover, $S(X)\otimes I$ and $I\otimes S(Y)$ commute, so we obtain

$$\begin{aligned}
U_{X\Box Y}(t) &= \exp(itS(X\Box Y))\\
&= \exp(it(S(X)\otimes I+I\otimes S(Y)))\\
&= \exp(it(S(X)\otimes I))\exp(it(I\otimes S(Y))\\
&= (\exp(itS(X))\otimes I)(I\otimes\exp(itS(Y)))\\
&= \exp(itS(X))\otimes\exp(itS(Y))\\
&= U_X(t)\otimes U_Y(t).
\end{aligned}$$

□

It follows from this lemma that if X has uniform mixing at time τ, and Y also has uniform mixing at time τ, then $X \square Y$ has uniform mixing at time τ. Similarly, if X has perfect state transfer between vertices a and b at time τ, and Y has perfect state transfer between vertices c and d at time τ, then $X \square Y$ has perfect state transfer between vertices (a,c) and (b,d) at time τ. Finally, if X is periodic at vertex a at time τ, and Y is periodic at vertex c at time τ, then $X \square Y$ is periodic at vertex (a,c) at time τ.

3.2 Perfect State Transfer and Periodicity

A characterization of periodicity at a vertex in terms of the eigenvalue support of that vertex was given by Godsil [30] in 2011, and used by Godsil [32, 33] to derive results on perfect state transfer the following year. In this section, we discuss the development of these results. We begin with the observation that perfect state transfer is symmetric, and that perfect state transfer implies periodicity; we reproduce the proof for completeness.

3.2.1 Lemma. *[32, 33] Let X be a graph and let a, b be vertices in X. If perfect state transfer from a to b takes place at time τ, then it also takes place from b to a. Further, X is periodic with period 2τ at both a and b.*

Proof. Suppose X has perfect state transfer from vertex a to vertex b at time τ. By definition, there exists a complex number γ with $|\gamma| = 1$ such that $U(\tau)\mathbf{e}_a = \gamma \mathbf{e}_b$. It follows that

$$\gamma^{-1}\mathbf{e}_a = U(-\tau)\mathbf{e}_b$$

as $U(\tau)^{-1} = U(-\tau)$. Taking the complex conjugate of both sides, we obtain $U(\tau)\mathbf{e}_b = \gamma \mathbf{e}_a$ as desired.

We then obtain periodicity at vertex a since

$$U(2\tau)\mathbf{e}_a = U(\tau)U(\tau)\mathbf{e}_a = U(\tau)\gamma\mathbf{e}_b = \gamma^2\mathbf{e}_a,$$

and similarly, we obtain periodicity at vertex b. □

This result can be used to demonstrate that if perfect state transfer occurs between vertices a and b and between vertices a and c, then $b = c$. The observation is due to Kay [37]; here we provide some additional details compared to the original proof.

3.2.2 Lemma. *[37] Let X be a graph and suppose X has perfect state transfer between both a and b and a and c. Then $b = c$.*

Proof. Suppose $b \neq c$. Let τ_B be the minimum time at which perfect state transfer occurs between vertices a and b and let τ_C be the minimum time at which perfect state transfer occurs between vertices a and c. Without loss of generality, assume that $0 < \tau_C < \tau_B$. By the previous lemma, we have that X is periodic at a at time $2\tau_C$. Consider the situation at time $|\tau_B - 2\tau_C|$. We have

$$U(\tau_B - 2\tau_C)\mathbf{e}_a = U(\tau_B)U(-2\tau_C)\mathbf{e}_a = U(\tau_B)\gamma\mathbf{e}_a = \gamma'\mathbf{e}_b,$$

applying the definitions of periodicity and perfect state transfer. Taking the complex conjugate of both sides, we obtain

$$U(-(\tau_B - 2\tau_C))\mathbf{e}_a = (\gamma')^{-1}\mathbf{e}_b.$$

Hence there is perfect state transfer between vertices a and b at time $|\tau_B - 2\tau_C| < \tau_B$, which contradicts the definition of τ_B. The result follows. □

Using the spectral decomposition, further tools can be developed for considering perfect state transfer. This treatment follows Chapter 9 of [20]. The first consideration is the following observations; we restate the proof for completeness.

3.2.3 Lemma. *[20] If X has spectral decomposition $\sum_r \theta_r E_r$ and $a, b \in V(X)$, then*

$$\begin{aligned} |U(t)_{a,b}| &\leq \sum_r |(E_r)_{a,b}| && (3.1)\\ &\leq \sum_r \sqrt{(E_r)_{a,a}}\sqrt{(E_r)_{b,b}} && (3.2)\\ &\leq \sqrt{\sum_r (E_r)_{a,a} \sum_r (E_r)_{b,b}} && (3.3)\\ &= 1. && (3.4) \end{aligned}$$

Proof. The first inequality is an application of the triangle inequality. The second inequality is an application of Cauchy-Schwarz, which states that for all vectors u and v, we have $|u^T v| \leq \|u\|\,\|v\|$. Hence, we take $u = E_r\mathbf{e}_a$ and $v = E_r\mathbf{e}_b$. The third inequality is also an application of Cauchy-Schwarz, where we take $u = (\sqrt{(E_r)_{a,a}})_r$ and $v = (\sqrt{(E_r)_{b,b}})_r$. Finally, it follows from the spectral decomposition that $\sum_r (E_r)_{a,a} = \sum_r (E_r)_{b,b} = 1$. □

The next consideration is the cases when the equality holds. Let σ_r denote the sign of $(E_r)_{a,b}$. The following result is demonstrated by Coutinho and Godsil [20]; we add a few details compared to their proof.

3.2.4 Lemma. *[20] The inequality $|U(t)_{a,b}| \leq \sum_r |(E_r)_{a,b}|$ holds with equality if and only if there is a complex number γ such that $e^{it\theta_r} = \gamma\sigma_r$ whenever $(E_r)_{a,b} \neq 0$. If equality holds at time t then $U(2t)_{a,b} = 0$.*

Proof. Since $|U(t)_{a,b}| = |\sum_r e^{it\theta_r} E_r|$, then equality is achieved in the triangle inequality if and only if $e^{it\theta_r}\sigma_r$ is constant, as desired. Then, we see that

$$U(2t)_{a,b} = \sum_r (e^{it\theta_r})^2 (E_r)_{a,b} = \sum_r \gamma^2 (E_r)_{a,b} = \gamma^2 \sum_r (E_r)_{a,b} = 0,$$

by applying the spectral decomposition. □

This result shown by Godsil [30] provides the following consequence in terms of the ratio condition, earlier versions of which are due to Saxena et al. [41] and Christandl et al. [17]. We say that the *ratio condition* holds at a vertex a if, for any four eigenvalues $\theta_k, \theta_\ell, \theta_r, \theta_s \in \Theta_a$ such that $\theta_r \neq \theta_s$, we have

$$\frac{\theta_k - \theta_\ell}{\theta_r - \theta_s} \in \mathbb{Q}.$$

The result is stated only for the forward direction in [30] and a sketch of the reverse direction is provided in [20]. We present the full details here.

3.2.5 Corollary. *[30] A graph X is periodic at the vertex a if and only if the ratio condition holds at a.*

Proof. By definition, if X is periodic at a at time t, then $|U(t)_{a,a}| = 1$, and so equality holds in each of the inequalities in Lemma 3.2.3. Hence, by Lemma 3.2.4, if $\theta_r \in \Theta_a$, then there is a complex number γ such that $e^{it\theta_r} = \gamma$ (as $(E_r)_{a,a} > 0$). Hence, we see that

$$1 = \frac{\gamma}{\gamma} = \frac{\exp(it\theta_k)}{\exp(it\theta_\ell)} = \exp(it(\theta_k - \theta_\ell)),$$

which implies that there exists an integer $m_{k,\ell}$ such that $t(\theta_k - \theta_\ell) = 2m_{k,\ell}\pi$. Hence, we see

$$\frac{\theta_k - \theta_\ell}{\theta_r - \theta_s} = \frac{t(\theta_k - \theta_\ell)}{t(\theta_r - \theta_s)} = \frac{2m_{k,\ell}\pi}{2m_{r,s}\pi} = \frac{m_{k,\ell}}{m_{r,s}} \in \mathbb{Q}.$$

Conversely, if the ratio condition holds at a, fix eigenvalues θ_1 and θ_2, and consider the ratios

$$r_{k,\ell} = \frac{\theta_k - \theta_\ell}{\theta_1 - \theta_2}$$

for all θ_k, θ_ℓ. Since X is finite, there exists an integer M such that $Mr_{k,\ell} \in \mathbb{Z}$ for all k, ℓ. Consider $\tau = \frac{2M\pi}{\theta_1 - \theta_2}$. Then we have

$$\tau(\theta_k - \theta_\ell) = \frac{2M\pi}{\theta_1 - \theta_2}(\theta_k - \theta_\ell) = 2Mr_{k,\ell}\pi,$$

which by definition of M, is an integer multiple of 2π. Hence, $\exp(i\tau(\theta_k - \theta_\ell)) = 1$, which implies there is a constant number γ such that $e^{i\tau\theta} = \gamma$. Thus,

$$U(\tau)_{a,a} = \sum_\theta e^{it\theta}(E_\theta)_{a,a} = \sum_\theta \gamma(E_\theta)_{a,a} = \gamma \sum_\theta (E_\theta)_{a,a} = \gamma,$$

which completes the proof. □

Analyzing the later inequalities of Lemma 3.2.3, a connection between pretty good state transfer and strongly cospectral vertices is obtained. The result was originally observed by Dave Witte Morris (as cited in [32]); we provide the following proof.

3.2.6 Lemma. *[32, private communication with Morris] If we have pretty good state transfer from a to b in X, then a and b are strongly cospectral vertices.*

Proof. By definition, if we have pretty good state transfer from a to b in X, then there exists a sequence of times $\{t_k\}$ such that

$$\lim_{k\to\infty} |U(t_k)_{a,b}| = 1.$$

By the first inequality of Lemma 3.2.3, we must have that $\sum_r |(E_r)_{a,b}| = 1$, and so the second and third inequalities must hold with equality. For the second, this implies that a and b are parallel, and for the third, this implies that a and b are cospectral. Then by Lemma 2.3.3, a and b are strongly cospectral. □

We have now presented the tools necessary to consider the following characterization of Godsil [30] of periodicity at a vertex. We provide an alternate presentation of the proof.

3.2.7 Theorem. *[30] Suppose X is a graph with at least two vertices. Then X is periodic at a if and only if either:*

a) The eigenvalues in Θ_a are integers.

b) There is a square-free integer Δ, the eigenvalues in Θ_a are quadratic integers in $\mathbb{Q}(\sqrt{\Delta})$, and the difference of any two eigenvalues in Θ_a is an integer multiple of $\sqrt{\Delta}$.

Proof. The sufficiency of either of the two stated conditions is clear from the ratio condition. It remains to prove their necessity. Assume X is periodic at a. We first assume that there are at least two eigenvalues in Θ_a, say θ_1 and θ_2, that are integers. Then for any other eigenvalue $\theta \in \Theta_a$, we have by the ratio condition that

$$\frac{\theta - \theta_1}{\theta_2 - \theta_1} \in \mathbb{Q}$$

from which it follows that θ is an integer, as required.

Now suppose at most one eigenvalue of Θ_a is an integer. Suppose $|\Theta_a| = 2$. Then at least one eigenvalue of $\Theta_a = \{\theta_1, \theta_2\}$, say θ_1, is not an integer (and moreover, is not rational). Since Θ_a contains all algebraic conjugates of θ_1 (by Corollary 2.4.2), it follows that θ_1 and θ_2 are roots of a quadratic polynomial, and hence the second condition is satisfied.

Now suppose $|\Theta_a| \geq 3$. By the ratio condition, we have

$$\theta_r - \theta_s = q_{r,s}(\theta_2 - \theta_1)$$

and hence

$$\prod_{r \neq s}(\theta_r - \theta_s) = (\theta_2 - \theta_1)^{|\Theta_a^2| - |\Theta_a|} \prod_{r \neq s} q_{r,s}.$$

Thus, we have

$$(\theta_2 - \theta_1)^{|\Theta_a^2| - |\Theta_a|} \in \mathbb{Q},$$

since the product on the left hand side of the previous equation is an integer, and the product of the $q_{r,s}$'s is rational. Moreover, the above expression is an integer since $\theta_2 - \theta_1$ is an algebraic integer. Now, suppose m is the least positive integer such that $(\theta_2 - \theta_1)^m$ is an integer. Then the conjugates of $\theta_2 - \theta_1$ are of the form $\beta \exp(2\pi i k/m)$. Since the eigenvalues of X are real, we see that $x \leq 2$. Hence it follows from the ratio condition that $(\theta_r - \theta_s)^2 \in \mathbb{Z}$ for all r, s.

Suppose $(\theta_2 - \theta_1)^2 = \Delta$. Then for each $\theta_r \in \Theta_a$, we have

$$\theta_r = \theta_r - \theta_1 + \theta_1 = q_{r,1}\sqrt{\Delta} + \theta_1$$

and so we obtain

$$|\Theta_a|\theta_1 - \sqrt{\Delta}\sum_r q_{r,1} = \sum_r \theta_r \in \mathbb{Z},$$

from which it follows that θ_1 is of the form $a + b_1\sqrt{\Delta}$, where $a, b_1 \in \mathbb{Q}$. Moreover, θ_1 is a quadratic integer. It follows that

$$\theta_r = a + (b_1 + q_{r,1})\sqrt{\Delta},$$

which completes the proof. □

In the Laplacian case, an even stronger result is obtained, as observed by Coutinho [23] in 2014 and extended by Countiho and Godsil [20]. We provide an alternative presentation.

3.2.8 Corollary. *[23, 20] Suppose X is a connected graph with at least two vertices and is periodic at a with respect to the Laplacian. Then $\Theta_a \subseteq \mathbb{Z}$.*

Proof. Suppose there exists $\theta \in \Theta_a$ such that $\theta \notin \mathbb{Z}$. By the previous theorem, θ is a quadratic integer, and so its conjugate $\overline{\theta}$ is also in Θ_a by Corollary 2.4.2. It is also clear that $0 \in \Theta_a$ is a simple eigenvector with eigenvector $\mathbf{1}$. Hence by the ratio condition we have

$$\frac{\theta}{\overline{\theta}} = \frac{\theta - 0}{\overline{\theta} - 0} \in \mathbb{Q},$$

which implies that $\overline{\theta} = -\theta$. However, all Laplacian eigenvalues are nonnegative, which implies $\theta = 0$, contradicting our initial assumption. Hence $\Theta_a \subseteq \mathbb{Z}$ as desired. □

We now discuss some of the consequences of this result. The first result follows immediately, as observed by Coutinho and Godsil [20], and can be used to show perfect state transfer is a fairly limited property, as demonstrated by Godsil [33]. We provide an alternative proof using the covering radius of a graph.

3.2.9 Corollary. *[20] If X is periodic at the vertex a then any two distinct elements of Θ_a differ by at least 1.*

3.2.10 Corollary. *[33] There are only finitely many connected graphs with maximum valency at most k where perfect state transfer relative to the adjacency matrix or Laplacian occurs.*

Proof. Let X be a connected graph with maximum valency at most k and with perfect state transfer between vertices a and b. By Corollary 3.2.9, we have $|\Theta_a| < 2k+1$, as all eigenvalues are contained in the interval $[-k, k]$. By Lemma 2.4.3, we have that the covering radius of a is at most $2k$. Hence, the number of vertices in the graph is bounded above by $k(k-1)^{2k-1}$, and the result follows. □

In the next section, we discuss applying these results on periodicity to perfect state transfer on trees.

3.3 Perfect State Transfer on Trees

Perfect state transfer was characterized with respect to the adjacency matrix for paths by Christandl et al. [17] in 2005 for the end vertices, and independently by Stevanović [44] and Godsil [32] in 2011 and 2012 for any pair of vertices. With respect to the Lapclain, perfect state transfer was characterized for trees by Coutinho and Liu [22] in 2015. The main focus of this section is a discussion of the development of these results. Our treatment follows Chapter 12 of [20]. We first introduce several spectral properties of paths that will be used throughout this work. The first consideration is the characteristic polynomial of a path; the following straightforward argument is included for completeness.

3.3.1 Theorem. *(e.g. [5]) The characteristic polynomial of a path is given by the following recurrence relation:*

$$\phi(P_n, x) = x\phi(P_{n-1}, x) - \phi(P_{n-2}, x), n \geq 2; \quad \phi(P_0, x) = 1,\ \phi(P_1, x) = x.$$

Proof. Let A_n denote the adjacency matrix for P_n. Calculating directly, we see that

$$\begin{aligned}\phi(P_n, x) &= \det(xI - A_n) \\ &= x\det(xI - A_{n-1}) - \det(xI - A_{n-2}) \\ &= x\phi(P_{n-1}, x) - \phi(P_{n-2}, x)\end{aligned}$$

as desired. Moreover, we see by direct calculation that $\phi(P_0, x) = 1$ and $\phi(P_1, x) = x$. □

The eigenvalues and eigenvectors of the path can now be calculated. The first step is to determine an expression for the following generating series. We present an alternate argument to that of Coutinho and Godsil [20] that does not use matrices.

3.3.2 Lemma. *[20]* $\sum_{n\geq 0} t^n \phi(P_n, x) = \frac{1}{1-xt-t^2}$.

Proof. Evaluating this expression, we obtain

$$\begin{aligned}I := \sum_{n\geq 0} t^n \phi(P_n, x) &= 1 + xt + \sum_{n\geq 2} t^n (x\phi(P_{n-1}, x) - \phi(P_{n-2}, x)) \\ &= 1 + xt + xt(I - 1) - t^2 I\end{aligned}$$

and therefore,

$$I := \sum_{n\geq 0} t^n \phi(P_n, x) = \frac{1}{1 - xt + t^2},$$

as desired. □

The output obtained from the characteristic polynomial for an input of a particular form is demonstrated; we provide additional details compared to the proof outlined by Countinho and Godsil [20].

3.3.3 Theorem. *[20]* $\phi(P_n, 2\cos(\zeta)) = \frac{\sin((n+1)\zeta)}{\sin(\zeta)}$.

Proof. We use partial fractions to evaluate the characteristic polynomials from the expression we previously derived. The roots are

$$\alpha = \frac{1}{2}\left(2\cos(\zeta) + \sqrt{4cos^2(\zeta) - 4}\right) = \cos(\zeta) + i\sin(\zeta) = e^{i\zeta}$$

$$\beta = \frac{1}{2}\left(2\cos(\zeta) - \sqrt{4cos^2(\zeta) - 4}\right) = \cos(\zeta) - i\sin(\zeta) = e^{-i\zeta}$$

and so we find

$$\frac{1}{1 - xt + t^2} = \frac{1}{\alpha - \beta}\left(\frac{\alpha}{1 - \alpha t} - \frac{\beta}{1 - \beta t}\right)$$

from which it follows that

$$\phi(P_n, 2\cos(\zeta)) = \frac{\alpha^{n+1} - \beta^{n+1}}{\alpha - \beta} = \frac{e^{(n+1)i\zeta} - e^{-(n+1)i\zeta}}{e^{i\zeta} - e^{-i\zeta}} = \frac{\sin((n+1)\zeta)}{\sin(\zeta)}$$

as desired. □

This result immediately implies the form of the roots of the characteristic polynomial, and hence the eigenvalues of P_n.

3.3.4 Corollary. *[20] The eigenvalues of P_n are*

$$2\cos\left(\frac{\pi k}{n+1}\right), \qquad 1 \leq k \leq n.$$

Proof. It follows that $2\cos(\zeta)$ is a zero of $\phi(P_n, x)$ if and only if $\sin((n+1)\zeta) = 0$. Hence, the eigenvalues of P_n are

$$2\cos\left(\frac{\pi k}{n+1}\right), \qquad 1 \leq k \leq n,$$

as desired. □

Moreover, an eigenvector corresponding to each eigenvalue can be calculated, and therefore so can the idempotents of the spectral decomposition of the adjacency matrix of P_n. We fill in a few details of the argument of Coutinho and Godsil [20].

3.3.5 Lemma. *[20] The idempotents $E_1, \dots, E_n$ in the spectral decomposition of P_n are given by*

$$(E_r)_{j,k} = \frac{2}{n+1} \sin\left(\frac{jr\pi}{n+1}\right) \sin\left(\frac{kr\pi}{n+1}\right).$$

Proof. We first compute eigenvectors of P_n. For $1 \leq r \leq n$, let $\beta_r = \pi r/(n+1)$ and $z(\beta_r) = \begin{pmatrix} \sin(\beta_r) & \sin(2\beta_r) & \cdots & \sin(n\beta_r) \end{pmatrix}^T$. We observe that

$$A \begin{pmatrix} \sin(\beta_r) \\ \sin(2\beta_r) \\ \vdots \\ \sin(n\beta_r) \end{pmatrix} = \begin{pmatrix} \sin(2\beta_r) \\ \sin(\beta_r) + \sin(3\beta_r) \\ \vdots \\ \sin((n-1)\beta_r) \end{pmatrix} = 2\cos(\beta_r) \begin{pmatrix} \sin(\beta_r) \\ \sin(2\beta_r) \\ \vdots \\ \sin(n\beta_r) \end{pmatrix} - \sin((n+1)\beta_r)\mathbf{e}_n$$

and so $z(\beta_r)$ is an eigenvector with eigenvalue $2\cos(\beta_r)$. It follows that each eigenvalue is simple and so

$$E_r = \frac{1}{z(\beta_r)^T z(\beta_r)} z(\beta_r) z(\beta_r)^T.$$

It remains to calculate the inner product $z(\beta_r)^T z(\beta_r)$. We have

$$\begin{aligned} z(\beta_r)^T z(\beta_r) &= \sum_{m=1}^{n} \sin^2(m\beta_r) \\ &= \sum_{m=0}^{n} \left(\frac{1}{2i}(e^{im\beta_r} - e^{-im\beta_r}) \right)^2 \\ &= -\frac{1}{4} \sum_{m=0}^{n} e^{2im\beta_r} - 2 + e^{-2im\beta_r} \\ &= \frac{n+1}{2} - \frac{1}{4} \left(\frac{1 - e^{2i(n+1)\beta_r}}{1 - e^{2i\beta_r}} + \frac{1 - e^{-2i(n+1)\beta_r}}{1 - e^{-2i\beta_r}} \right) = \frac{n+1}{2}, \end{aligned}$$

since $2(n+1)\beta$ is an even multiple of π. □

We next derive the following observation regarding the eigenvalue support of a vertex of P_n. The result has been observed previously without being explicitly stated. We provided a proof in our work in [45]; we give a simplified version here using the explicit form of the idempotents for completeness.

3.3.6 Lemma. *The eigenvalue support of vertex a of the graph P_n is given by*

$$\Theta_a = \{\theta_j : n+1 \nmid aj\}.$$

Proof. Suppose first that $n+1 \mid aj$. We consider the (c, a) entry of E_j for each vertex c:

$$(E_j)_{(c,a)} = \frac{2}{n+1}\left(\sin\frac{cj\pi}{n+1}\right)\left(\sin\frac{aj\pi}{n+1}\right) = 0.$$

It therefore follows that $E_j\mathbf{e}_a = 0$, so $\theta_j \notin \Theta_a$.

Now suppose that $n+1 \nmid aj$. We consider the (a, a) entry of E_j.

$$(E_j)_{(a,a)} = \frac{2}{n+1}\left(\sin\frac{aj\pi}{n+1}\right)^2$$

Since $\sin x = 0$ if and only if x is an integer multiple of π and $aj/(n+1)$ is not integral, it follows that $(E_j)_{(a,a)} \neq 0$, and hence $E_j\mathbf{e}_a \neq 0$, so $\theta_j \in \Theta_a$. □

We further characterize which pairs of vertices of a path are strongly cospectral as a straightforward consequence; it is typically observed without being explicitly proven. Here we provide a proof for completeness.

3.3.7 Lemma. *For the graph P_n, vertices a and b are strongly cospectral if and only if $a+b = n+1$. Moreover, when a and b are strongly cospectral, $E_r\mathbf{e}_a = (-1)^{r+1}E_r\mathbf{e}_b$.*

Proof. If $a+b = n+1$, then by the previous lemma, for $c \in V(P_n)$, we have

$$\begin{aligned}
(E_r)_{a,c} &= \frac{2}{n+1}\sin\left(\frac{ar\pi}{n+1}\right)\sin\left(\frac{cr\pi}{n+1}\right) \\
(E_r)_{b,c} &= \frac{2}{n+1}\sin\left(\frac{(n+1-a)r\pi}{n+1}\right)\sin\left(\frac{cr\pi}{n+1}\right) \\
&= \frac{2}{n+1}\left(\sin(r\pi)\cos\left(\frac{ar\pi}{n+1}\right) - \cos(r\pi)\sin\left(\frac{ar\pi}{n+1}\right)\right)\sin\left(\frac{cr\pi}{n+1}\right) \\
&= (-1)^{r+1}(E_r)_{a,c},
\end{aligned}$$

and so $E_r\mathbf{e}_a = (-1)^{r+1}E_r\mathbf{e}_b$ as desired.

Conversely, suppose a and b are strongly cospectral, then $E_r\mathbf{e}_a = \pm E_r\mathbf{e}_b$ for all r. Then for all $c \in V(P_n)$, we have we have

$$(E_1)_{a,c} = \pm(E_1)_{b,c}$$
$$\frac{2}{n+1}\sin\left(\frac{a\pi}{n+1}\right)\sin\left(\frac{c\pi}{n+1}\right) = \pm\frac{2}{n+1}\sin\left(\frac{b\pi}{n+1}\right)\sin\left(\frac{c\pi}{n+1}\right)$$
$$\sin\left(\frac{a\pi}{n+1}\right) = \pm\sin\left(\frac{b\pi}{n+1}\right)$$
$$a = n+1-b$$

as desired. □

We now present the characterization of perfect state transfer on paths with respect to the adjacency matrix. We provide an alternative proof making use of covering radius and the ratio condition.

3.3.8 Theorem. *[44, 32] If $n \geq 4$, perfect state transfer does not occur on P_n.*

Proof. Suppose perfect state transfer occurs on P_n between vertices a and b. Then P_n is periodic at a. By Corollary 3.2.9, any two distinct elements of Θ_a differ by at least 1. By Corollary 3.3.4, the eigenvalues of P_n are in the interval $(-2,2)$, and hence there can be at most four eigenvalues in Θ_a. By Lemma 2.4.3, the covering radius is at most three. Hence $n \leq 6$, since only one vertex in P_7 has covering radius at most three, and every vertex in a longer path has covering radius at least four.

In P_6, the only vertices with covering radius at most three are vertices 3 and 4. So if there is perfect state transfer between vertices 3 and 4, then we have $U(t)\mathbf{e}_3 = \gamma\mathbf{e}_4$ and $U(t)\mathbf{e}_4 = \gamma\mathbf{e}_3$ for some time t and complex number γ. So we have

$$U(t)(\mathbf{e}_2 + \mathbf{e}_4) = U(t)A\mathbf{e}_3 = AU(t)\mathbf{e}_3 = \gamma A\mathbf{e}_4 = \gamma(\mathbf{e}_3 + \mathbf{e}_5),$$

using the fact that A and $U(t)$ commute. Hence, from the above equation, it follows that $U(t)\mathbf{e}_2 = \gamma\mathbf{e}_5$, which implies that there is perfect state transfer between vertices 2 and 5, but these vertices each have covering radius of four, a contradiction.

In P_5, the only vertices with covering radius at most three are vertices 2, 3, and 4, and we can rule out the middle vertex since it is not part of a cospectral pair. So if there is perfect state transfer between vertices 2 and 4, P_5 must be periodic at vertex 2. But eigenvalues $\sqrt{3}, 1, -1, -\sqrt{3}$ are all in the eigenvalue support of vertex 2, and

$$\frac{\sqrt{3}-(-\sqrt{3})}{1-(-1)} = \sqrt{3} \notin \mathbb{Q},$$

which contradicts the ratio condition, and hence we do not have perfect state transfer in P_5.

In P_4, all the vertices have covering radius at most three. The eigenvalues of P_4 are

$$\theta_1 = \frac{1}{2}(\sqrt{5}+1), \quad \theta_2 = \frac{1}{2}(\sqrt{5}-1), \quad \theta_3 = \frac{1}{2}(-\sqrt{5}+1), \quad \theta_4 = \frac{1}{2}(-\sqrt{5}-1)$$

and each is in the eigenvalue support of every vertex. Testing the ratio condition, we find

$$\frac{\theta_1-\theta_4}{\theta_2-\theta_3} = \frac{\sqrt{5}+1}{\sqrt{5}-1} = \frac{6+2\sqrt{5}}{4} \notin \mathbb{Q}.$$

Hence we do not have perfect state transfer on P_4, which completes the proof. □

The question of whether there are additional examples of perfect state transfer on trees remains open.

We now proceed to the Laplacian case. Even more can be said for this Hamiltonian; Coutinho and Liu [22] demonstrated that with the exception of P_2, we cannot have perfect state transfer on trees. We outline their approach in what follows. As a first step, the phase factor required for Laplacian perfect state transfer is stated; the straightforward argument is included for completeness.

3.3.9 Lemma. *[20] If $U(t)$ is the transition matrix relative to the Laplacian of a graph and we have perfect state transfer between vertices a and b at time τ, then $U(\tau)\mathbf{e}_a = \mathbf{e}_b$.*

Proof. By definition of perfect state transfer, we have that $U(\tau)\mathbf{e}_a = \gamma\mathbf{e}_b$. We observe the following

$$\gamma = \gamma\mathbf{1}^T\mathbf{e}_b = \mathbf{1}^T U(\tau)\mathbf{e}_a = \mathbf{1}\mathbf{e}_a = 1,$$

using the fact that $\mathbf{e}_a$ and $\mathbf{e}_b$ are elementary vectors and that $\mathbf{1}$ is an eigenvector for $U(t)$ with eigenvalue 1. □

It is next shown that there is an eigenvalue of each sign in the eigenvalue support of each vertex of a pair of strongly cospectral vertices, and the cases when equality holds are characterized. Two vertices a and b are said to be *twins* if either $N(a) = N(b)$ or $N[a] = N[b]$, i.e. a and b have the same open or closed neighbourhood. We outline the proof for completeness.

3.3.10 Lemma. *[22] Suppose a and b are vertices in the connected graph X that are strongly cospectral, relative to the Laplacian. Then there is at least one eigenvalue θ in Θ_a such that $\sigma_\theta = 1$ and at least one eigenvalue ρ in Θ_a such that $\sigma_\rho = -1$. If there is only one such eigenvalue such that $\sigma_\theta = 1$, then $|V(X)| = 2$; if there is only one such eigenvalue such that $\sigma_\rho = -1$, then a and b are twins.*

Proof. Consider the vectors

$$z^+ = \sum_{\substack{\theta\in\Theta_a \\ \sigma_\theta=1}} E_\theta \mathbf{e}_a, \qquad z^- = \sum_{\substack{\theta\in\Theta_a \\ \sigma_\theta=-1}} E_\theta \mathbf{e}_a.$$

We see that $z^+ + z^- = \mathbf{e}_a$ (by spectral decomposition) and $z^+ - z^- = \mathbf{e}_b$ (by strong cospectrality). Hence we obtain the equivalent expressions

$$z^+ = \frac{1}{2}(\mathbf{e}_a + \mathbf{e}_b), \qquad z^- = \frac{1}{2}(\mathbf{e}_a - \mathbf{e}_b).$$

Moreover, we know that $\mathbf{1}$ is an eigenvector with eigenvalue 0, confirming there is at least one eigenvalue $\theta \in \Theta_a$ such that $\sigma_\theta = 1$. If this is the only such eigenvalue, then $\mathbf{e}_a + \mathbf{e}_b$ must also be an eigenvector with eigenvalue 0, so it follows from the fact that X is connected that $|V(X)| = 2$.

Now, as $z^- \neq 0$, it follows that there is at least one eigenvalue $\theta \in \Theta_a$ such that $\sigma_\theta = -1$. If there is only one such eigenvalue, then z^- must be an eigenvector. Hence we see that if $c \neq a, b$, then c is adjacent to a if and only if c is adjacent to b, and it follows that a and b are twins as desired. □

Next, the signs of the idempotents required to permit perfect state transfer are determined. Coutinho and Liu [22] present this result as a well known fact; we provide the following explicit proof.

3.3.11 Lemma. *[22] Suppose we have perfect state transfer between vertices a and b relative to the Laplacian. Let g be the gcd of the elements in Θ_a. If $\lambda \in \Theta_a$, then $\sigma_\lambda = 1$ if and only if λ/g is even.*

Proof. Since we have perfect state transfer between vertices a and b, then by Lemma 3.2.4, there is a complex number γ such that $e^{it\theta} = \gamma\sigma_\theta$ for all $\theta \in \Theta_a$. As the eigenvalues of Θ_a are integers by Corollary 3.2.8, then we have

$$\gamma\sigma_\theta = e^{it\theta} = (e^{itg})^{\theta/g}$$

For $\theta = 0$, we have $\sigma_0 = 1$, and hence $\gamma = 1$. Since by the previous lemma, there is at least one eigenvalue such that $\sigma_\theta = -1$, it follows that $e^{itg} = -1$, and hence the result follows. □

Now, for trees with an odd number of vertices, Laplacian perfect state transfer can be ruled out. The result makes use of the Matrix-Tree Theorem (see [35, Theorem 13.2.1]); the proof is outlined for completeness.

3.3.12 Theorem (Matrix-Tree Theorem)**.** *Let X be a graph on n vertices, and u be any of its vertices. Let $L[u]$ denote the submatrtix of L obtained by deleting the row and column indexed by u. Then the number of spanning trees of X is equal to* $\det L[u]$.

3.3.13 Lemma. *[22] If X is a graph with an odd number of vertices and an odd number of spanning trees, then Laplacian perfect state transfer does not occur on X.*

Proof. Suppose X has Laplacian perfect state transfer between vertices a and b. By Lemma 3.3.11, every eigenvalue λ such that $\sigma_\lambda = 1$ must be even. It is a straightforward consequence of the Matrix-Tree Theorem that the number of spanning trees of a graph is the product of the nonzero eigenvalues of the Laplacian. Hence, all non-zero eigenvalues are odd, so there is only one eigenvalue λ such that $\sigma_\lambda = 1$. Hence, by Lemma 3.3.10, $|V(X)| = 2$, contradicting that X has an odd number of vertices. □

Now, trees with an even number of vertices must be considered. Coutinho and Liu [22] provided the following stronger result; we provide an alternate presentation of their proof.

3.3.14 Theorem. *[22] Let X be a connected graph and assume that the number of spanning trees in X is a power of two. If there is Laplacian perfect state transfer from a to b in X, then there is precisely one eigenvalue θ in Θ_a such that $\sigma_\theta = -1$.*

Proof. Suppose λ is an eigenvalue of X with $\sigma_\lambda = -1$. Suppose further that p is an odd prime divisor of λ. Let v be an integral eigenvector of λ such that the gcd of its entries is 1. We observe that

$$Ly \equiv 0 \pmod{p}.$$

Moreover, we have that $y \equiv k\mathbf{1}$ for some integer k, as $\mathbf{1}$ is also in the kernel of L and the kernel has dimension 1, which follows from the number of spanning trees being a power of two. Using the fact that $\sigma_\lambda = -1$, we have that $y_a = -y_b$, from which we obtain $0 = y_a + y_b = 2k \pmod{p}$. Thus, we see that $k \equiv 0 \pmod{p}$, contradicting our choice of y. It follows that every eigenvalue λ such that $\sigma_\lambda = -1$ is a power of two, so by Lemma 3.3.11, there is only one such eigenvalue. □

With the previous results, the proof that there is only one tree with Laplacian perfect state transfer can be completed; we provide the following more detailed explanation.

3.3.15 Theorem. *[22] If T is a tree with more than two vertices, then we cannot have perfect state transfer on T relative to the Laplacian.*

Proof. Suppose T has Laplacian perfect state transfer between vertices a and b. By Lemma 3.3.13, T has an even number of vertices, and by Theorem 3.3.14, there is precisely one eigenvalue $\theta \in \Theta_a$ such that $\sigma_\theta = -1$, from which it follows by Lemma 3.3.10 that a and b are twins. Since T is a tree, it follows that a and b have valency one, and a common neighbour c. We observe that $\mathbf{e}_a - \mathbf{e}_b$ is an eigenvector with eigenvalue 1, and $\sigma_1 = -1$.

From the proof of Lemma 3.3.10, we saw that

$$\sum_{\substack{\theta \in \Theta_a \\ \sigma_\theta = 1}} E_\theta \mathbf{e}_a = \frac{1}{2}(\mathbf{e}_a + \mathbf{e}_b)$$

and so we obtain

$$\sum_{\substack{\theta \in \Theta_a \\ \sigma_\theta = 1}} \mathbf{e}_a^T E_\theta \mathbf{e}_a = \frac{1}{2},$$

$$\sum_{\substack{\theta \in \Theta_a \\ \sigma_\theta = 1}} \mathbf{e}_c^T E_\theta \mathbf{e}_a = 0.$$

We also have that $L\mathbf{e}_a = \mathbf{e}_a - \mathbf{e}_c$, which gives $\mathbf{e}_c = (I - L)\mathbf{e}_a$. Hence, for each eigenvalue θ, we obtain

$$\mathbf{e}_c^T E_\theta \mathbf{e}_a = \mathbf{e}_a^T (I - L) E_\theta \mathbf{e}_a = (1 - \theta)\mathbf{e}_a^T E_\theta \mathbf{e}_a.$$

Applying the fact that every eigenvalue in $\Theta_a \setminus \{0, 1\}$ is at least two, we obtain

$$0 = \sum_{\substack{\theta \in \Theta_a \\ \sigma_\theta = 1}} \mathbf{e}_c^T E_\theta \mathbf{e}_a = \sum_{\substack{\theta \in \Theta_a \\ \sigma_\theta = 1}} (1 - \theta)\mathbf{e}_a^T E_\theta \mathbf{e}_a \leq \sum_{\substack{\theta \in \Theta_a \\ \sigma_\theta = 1}} \mathbf{e}_a^T E_\theta \mathbf{e}_a + \frac{2}{n} = -\frac{1}{2} + \frac{2}{n}.$$

Hence we see that $n \leq 4$, so $n = 4$.

It remains to verify that $K_{1,3}$ does not have Laplacian perfect state transfer. The spectral decomposition of $L(K_{1,3})$ is given by

$$E_0 = \begin{pmatrix} 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{pmatrix},$$

$$E_1 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 2/3 & -1/3 & -1/3 \\ 0 & -1/3 & 2/3 & -1/3 \\ 0 & -1/3 & -1/3 & 2/3 \end{pmatrix},$$

$$E_4 = \begin{pmatrix} 3/4 & -1/4 & -1/4 & -1/4 \\ -1/4 & 1/12 & 1/12 & 1/12 \\ -1/4 & 1/12 & 1/12 & 1/12 \\ -1/4 & 1/12 & 1/12 & 1/12 \end{pmatrix};$$

from which it is clear that no pair of vertices in $K_{1,3}$ are strongly cospectral, completing the proof. □

3.4 Future Directions

Perfect state transfer with respect to the adjacency matrix has been characterized for paths but remains open for trees. On the other hand, perfect state transfer with respect to the Laplacian has been completely characterized for trees. We are interested in resolving trees for the adjacency matrix. Fan and Godsil investigated perfect and pretty good state transfer on *double stars*, denoted $S_{k,l}$, which is formed by joining the non-leaf vertices of $K_{1,k}$ and $K_{1,\ell}$ by an edge, and determined that these graphs never have perfect state transfer.

For both perfect state transfer and pretty good state transfer, the vertices involved are required to be strongly cospectral. It would be interesting to determine if there is a tree with a set of three vertices, each pair of which are strongly cospectral. However, we note by Lemma 3.2.2 that it is not possible to have perfect or pretty good state transfer between each pair of vertices, so such a tree is unlikely to provide insight to state transfer.

Chapter 4

Pretty Good State Transfer on Paths

As we have seen, examples of perfect state transfer are relatively rare, and the notion of pretty good state transfer was isolated by multiple authors (see Godsil [32], for example) as a relaxation of perfect state transfer. Formally, a graph X is said to have *pretty good state transfer* between vertices a and b if, there exist sequences of times $\{\tau_k\}$ of real numbers and $\{\gamma_k\}$ of complex numbers with $|\gamma_k| = 1$, such that

$$\lim_{k\to\infty} \|U(\tau_k)\mathbf{e}_a - \gamma_k \mathbf{e}_b\| = 0,$$

or equivalently, for every $\epsilon > 0$, there exist $\tau_\epsilon \in \mathbb{R}$ and $\gamma_\epsilon \in \mathbb{C}$ with $|\gamma_\epsilon| = 1$, such that

$$\|U(\tau_\epsilon)\mathbf{e}_a - \gamma_\epsilon \mathbf{e}_b\| < \epsilon.$$

This definition is often presented using a fixed γ. We demonstrate that these two definitions are equivalent.

4.0.1 Proposition. *There exist sequences of times $\{\tau_k\}$ of real numbers and $\{\gamma_k\}$ of complex numbers with $|\gamma_k| = 1$, such that*

$$\lim_{k\to\infty} \|U(\tau_k)\mathbf{e}_a - \gamma_k \mathbf{e}_b\| = 0, \tag{A}$$

if and only if there exist a sequence of times $\{\tau_\ell\}$ of real numbers and a complex number γ with $|\gamma| = 1$, such that

$$\lim_{k\to\infty} \|U(\tau_\ell)\mathbf{e}_a - \gamma \mathbf{e}_b\| = 0, \tag{B}$$

Proof. It is clear that if (B) holds, then (A) also holds taking $\tau_k = \tau_\ell$ and $\gamma_k = \gamma$. It remains to show that (A) implies (B). Since the set of complex numbers of norm 1 is bounded, there exists a convergent subsequence $\{\gamma_\ell\}$ of γ_k which converges to some γ with $|\gamma| = 1$. Hence, for every $\epsilon > 0$, there exists a $j \in \mathbb{N}$ such that $\|U(\tau_j)\mathbf{e}_a - \gamma_j \mathbf{e}_b\| < \epsilon/2$ and $|\gamma_j - \gamma| < \epsilon/2$. Thus we have

$$\begin{aligned}\|U(\tau_j)\mathbf{e}_a - \gamma\mathbf{e}_b\| &= \|U(\tau_j)\mathbf{e}_a - \gamma_j\mathbf{e}_b + \gamma_j\mathbf{e}_b - \gamma\mathbf{e}_b\| \\ &\leq \|U(\tau_j)\mathbf{e}_a - \gamma_j\mathbf{e}_b\| + |\gamma_j - \gamma|\,\|\mathbf{e}_b\| \\ &< \epsilon/2 + \epsilon/2 \\ &= \epsilon,\end{aligned}$$

so (B) holds as desired. □

The focus of this chapter is to fully characterize pretty good state transfer of single vertices on paths, both for the adjacency matrix model and the Laplacian model. The results for the adjacency matrix model have been previously published in [21, 45]. We first examine properties of the transition matrix, and demonstrate that graphs are *almost periodic*, which addresses the case of pretty good state transfer when the vertices coincide.

4.1 Almost Periodicity

We say a graph X is *almost periodic* if there exist sequences of times $\{\tau_k\}$ of real numbers and $\{\gamma_k\}$ of complex numbers with $|\gamma_k| = 1$ such that

$$\lim_{k\to\infty} \|U(\tau_k) - \gamma_k I\| = 0,$$

or equivalently, for every $\epsilon > 0$, there exist $\tau_\epsilon \in \mathbb{R}$ and $\gamma_\epsilon \in \mathbb{C}$ with $|\gamma_\epsilon| = 1$ such that

$$\|U(\tau_\epsilon) - \gamma_\epsilon I\| < \epsilon.$$

Using the fact that trigonometric polynomials, i.e. functions of the form

$$\sum_r a_r \exp(i\theta_r t),$$

are almost periodic (see Section 2.5), we observe that the entries of a transition matrix $U(t)$ with any finite Hermitian matrix as the Hamiltonian is almost periodic. Moreover, a compactness argument yields that $U(t)$ is almost periodic in $\mathbb{C}^{n\times n}$.

4.1.1 Proposition. *Let H be finite and Hermitian, and let $U(t) = \exp(itH)$. Then $U(t)$ is almost periodic.*

Proof. As H is finite and Hermitian, we can obtain the spectral decomposition of H as

$$H = \sum_r \theta_r E_r,$$

and hence we can write

$$U(t) = \sum_r \exp(it\theta_r) E_r.$$

Since the entries of $U(t)$ are trigonometric polynomials, they are almost periodic. It follows by compactness that $U(t)$ is almost periodic, which completes the proof. □

It follows immediately that every graph is almost periodic.

4.1.2 Corollary. *Every graph X is almost periodic.*

Proof. Let $U(t)$ be a transition matrix for X. By Proposition 4.1.1, $U(t)$ is almost periodic. Hence, by definition, for every $\epsilon > 0$, there exists a τ such that $\|U(t+\tau) - U(t)\| \leq \epsilon$. Since $U(0) = I$, we have that $\|U(\tau) - I\| \leq \epsilon$, as desired. □

Hence, when considering pretty good state transfer between vertices a and b, we need not consider the case when $a = b$, as this property trivially holds as demonstrated above.

4.2 Between the End Vertices

We begin our consideration of pretty good state transfer on paths by considering the following example.

4.2.1 Example. Suppose we wish to verify whether P_4 has pretty good state transfer between its end vertices. By definition, we have

$$\|U(\tau)\mathbf{e}_1 - \gamma\mathbf{e}_4\| < \epsilon$$

and using spectral decomposition, we obtain

$$\left\| \left(\sum_{\theta_j \in \Theta_1} \exp(i\tau\theta_j)(E_j)\mathbf{e}_1 \right) - \gamma\mathbf{e}_4 \right\| < \epsilon.$$

Applying the observation that $E_r\mathbf{e}_1 = E_r\mathbf{e}_4$ when r is odd and $E_r\mathbf{e}_1 = -E_r\mathbf{e}_4$ when r is even, and letting $\gamma = \exp(i\delta)$, we have

$$\left\| \sum_{\theta_j \in \Theta_1} \big(\exp(i\tau\theta_j) - (-1)^{j+1}\exp(i\delta)\big) E_j\mathbf{e}_4 \right\| < \epsilon,$$

from which it follows that we desire

$$|\tau\theta_j - (\delta + \sigma_r\pi)| < \epsilon' \pmod{2\pi}, \quad (r : \theta_r \in \Theta_1), \tag{$*$}$$

where σ_r is even if r is odd and odd if r is even.

By $(*)$, it suffices to demonstrate a solution to the following system of inequalities

$$\left| \frac{\sqrt{5}+1}{2}\tau - \delta \right| < \epsilon \pmod{2\pi},$$

$$\left| \frac{\sqrt{5}-1}{2}\tau - \delta + \pi \right| < \epsilon \pmod{2\pi},$$

$$\left| \frac{-\sqrt{5}+1}{2}\tau - \delta \right| < \epsilon \pmod{2\pi},$$

$$\left| \frac{-\sqrt{5}-1}{2}\tau - \delta + \pi \right| < \epsilon \pmod{2\pi}.$$

By choosing $\delta = \pi/2$, we observe that the first and last inequalities and second and third inequalities differ only by a factor of -1. Hence, we have the system

$$\left| \frac{\sqrt{5}+1}{2}\tau - \frac{\pi}{2} \right| < \epsilon \pmod{2\pi}, \qquad \left| \frac{\sqrt{5}-1}{2}\tau + \frac{\pi}{2} \right| < \epsilon \pmod{2\pi}.$$

To apply Kronecker's Theorem, we need to consider all pairs of integers ℓ_1, ℓ_2 such that

$$\frac{\sqrt{5}+1}{2}\ell_1 + \frac{\sqrt{5}-1}{2}\ell_2 = 0.$$

Rearranging, we obtain

$$-\frac{\ell_2}{\ell_1} = \frac{\sqrt{5}+1}{\sqrt{5}-1} = \frac{3+\sqrt{5}}{2}$$

and observe that the left-most expression is rational, but the right-most expression is irrational; a contradiction which demonstrates there are no pairs of integers ℓ_1, ℓ_2 satisfying the equation. Hence our system of inequalities has a solution by Kronecker's Theorem (Theorem 2.5.1), and so P_4 has pretty good state transfer between its end vertices. $\diamondsuit$

In 2007, Burgarth [8] studied the problem of pretty good state transfer on paths using the Laplacian matrix as the Hamiltonian. Unfortunately, as pointed out by Banchi et al. [4], Burgarth's claim that pretty good state transfer would occur in all chains of prime length is false, as the symmetry used to demonstrate the claim was not entirely accurate. Vinet and Zhedanov [47] studied this problem under the term *almost perfect state transfer* in 2012. They established that pretty good state transfer occurred in paths when the eigenvalues of the Hamiltonian were linearly independent over the rational numbers. Around the same time, Godsil, Kirkland, Severini, and Smith [34] demonstrated the following result for pretty good state transfer on paths.

4.2.2 Theorem. *[34] There is pretty good state transfer between the end vertices of P_n with respect to the adjacency matrix if and only if:*

a) $n = 2^t - 1,\ t \in \mathbb{Z}_+$*;*

b) $n = p - 1,\ \ p$ *a prime; or*

c) $n = 2p - 1,\ \ p$ *a prime.*

Moreover, when pretty good state transfer occurs between the end vertices of P_n, then it occurs between vertices a and $n + 1 - a$ for all $a \neq (n + 1)/2$.

Further, Banchi et al. [4] demonstrated the analogous result for pretty good state transfer on paths in the Laplacian case in 2017.

4.2.3 Theorem. *[4] There is pretty good state transfer between the end vertices of P_n with respect to the Laplacian if and only if n is a power of 2. Moreover, in these cases, pretty good state transfer occurs between vertices a and $(n + 1 - a)$ for all $j = 1, \ldots, n$.*

However, neither result considers if pretty good state transfer is possible between internal vertices of a path when it is not possible between the end vertices. In fact, the former result is often misrepresented in the literature as completely characterizing pretty good state transfer on paths. In an earlier draft of their paper, Banchi et al. [4] flagged this discrepency, and presented as an open problem pretty good state transfer internal vertices under both models. In the following two sections, we will resolve these questions. The key observation is that while all eigenvalues are in the eigenvalue supports of the end vertices, this need not be the case for internal vertices, which reduces the number of inequalities to consider when applying Kronecker's Theorem. We will make use of the following result due to Banchi et al. [4]; we present a more detailed proof verifying this result.

4.2.4 Theorem. *[4] Let a and b be vertices of a graph X. Then pretty good state transfer occurs between a and b if and only if both conditions below are satisfied.*

a) Vertices a and b are strongly cospectral, in which case let $\zeta_j = (1-\sigma_j)/2$.

b) If there is a set of integers $\{\ell_j\}$ such that

$$\sum_{\theta_j \in \Theta_a} \ell_j \theta_j = 0 \quad \textit{and} \quad \sum_{\theta_j \in \Theta_a} \ell_j \zeta_j \textit{ is odd,}$$

then

$$\sum_{\theta_j \in \Theta_a} \ell_j \neq 0.$$

Proof. First suppose the two conditions are satisfied. We consider the system of inequalities

$$|\theta_j \tau - (\delta + \zeta_j \pi)| < \epsilon \pmod{2\pi}, \qquad (\theta_j \in \Theta_a).$$

Let $\{\ell_j\}$ be a set of integers such that

$$\sum_{\theta_j \in \Theta_a} \ell_j \theta_j = 0.$$

Then we desire

$$\sum_{\theta_j \in \Theta_a} \ell_j (\delta + \zeta_j \pi) \equiv 0 \pmod{2\pi}. \tag{\dagger}$$

We need to show that there exists a δ such that the above equation is true for all sets $\{\ell_j\}$. If $\sum \ell_j \zeta_j$ is even for every set of integers $\{\ell_j\}$, then we may choose $\delta = 0$. Otherwise, suppose for some set of integers $\{\ell_j\}$ that $\sum \ell_j \zeta_j$ is odd, in which case $\alpha := \sum \ell_j \neq 0$, and let δ be such that the above equation is satisfied for this set. Suppose $\{\ell'_j\}$ is also a set of integers such that

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell'_j \theta_j = 0.$$

Define $\alpha' = \sum \ell'_j$, and let 2^r be the largest power of 2 that divides α, 2^s be the largest power of 2 that divides α', and $t = \min\{r, s\}$. Take $\delta = \pi 2^{-r}$. Then we construct the set of integers $\gamma_j = 2^{-t}(\alpha' \ell_j - \alpha \ell'_j)$. It is a straightforward calculation that $\sum \gamma_j \theta_j = 0$ and $\sum \gamma_j = 0$. Now consider the expression

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \gamma_j \zeta_j = \sum_{\theta_j \in \Theta_{\mathbf{v}}} 2^{-t}(\alpha' \ell_j - \alpha \ell'_j)\zeta_j = \left(2^{-t}\alpha'\right) \left(\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j \zeta_j \right) - \left(2^{-t}\alpha\right) \left(\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell'_j \zeta_j \right).$$

We observe that $\sum \gamma_j \zeta_j$ is even, as otherwise we have a contradiction to our hypothesis, $\sum \ell_j \zeta_j$ is odd by our assumption, and at least one of $2^{-t}\alpha$ and $2^{-t}\alpha'$ is odd. If $2^{-t}\alpha'$ is odd, then both $2^{-t}\alpha$ and $\sum \ell'_j \zeta_j$ are odd, so $r = s$, and (†) is satisfied. Otherwise, $2^{-t}\alpha'$ is even, so $s > r$, $2^{-t}\alpha$ is odd and $\sum \ell'_j \zeta_j$ is even; thus (†) is satisfied. Therefore, by Kronecker's Theorem, the system of inequalities

$$|\theta_j \tau - (\delta + \zeta_j \pi)| < \epsilon \pmod{2\pi}, \qquad (\theta_j \in \Theta_a)$$

admits a solution τ_0 for τ. Hence we obtain

$$U(\tau_0) = \sum_{\theta_j \in \Theta_a} e^{i\tau_0 \theta_j} E_j = \sum_{\theta_j \in \Theta_a} (1 - \epsilon') e^{i\delta} \sigma_j E_j$$

and so $U(\tau_0)\mathbf{e}_a \approx e^{i\delta}\mathbf{e}_b$, and hence we have pretty good state transfer between vertices a and b.

Conversely, suppose pretty good state transfer occurs between a and b. By Lemma 3.2.6, a and b are strongly cospectral. Moreover, for some τ, we see that,

$$\begin{aligned} U(\tau)\mathbf{e}_a &\approx e^{i\delta}\mathbf{e}_b, \\ e^{i\theta_j \tau} E_j \mathbf{e}_a &\approx e^{i\delta} E_j \mathbf{e}_b, && (\theta_j \in \Theta_a), \\ e^{i\theta_j \tau} E_j \mathbf{e}_a &\approx (-1)^{j+1} e^{i\delta} E_j \mathbf{e}_b, && (\theta_j \in \Theta_{\mathbf{v}}), \\ \theta_j \tau &\approx \delta + \zeta_j \pi \pmod{2\pi}, && (\theta_j \in \Theta_a). \end{aligned}$$

So by Kronecker's Theorem, for every set of integers $\{\ell_j\}$ such that $\sum \ell_j \theta_j = 0$, we have

$$\sum_{\theta_j \in \Theta_a} \ell_j (\delta + \zeta_j \pi) \equiv 0 \pmod{2\pi}.$$

It follows that if $\sum \ell_j \zeta_j$ is odd, then $\sum \ell_j$ cannot be zero, or the above condition is not satisfied, which completes the proof. □

4.3 Adjacency Matrix Model

We begin our investigation of pretty good state transfer of internal vertices of paths under the adjacency matrix model by demonstrating an infinite family of paths with pretty good state transfer between internal vertices; the result can be found in the 2017 work of Coutinho, Guo, and van Bommel [21].

4.3.1 Theorem. *Given any odd prime p and positive integer t, there is pretty good state transfer in $P_{2^t p-1}$ between vertices a and $2^t - a$, whenever a is a multiple of 2^{t-1}.*

Proof. For simplicity, let $n = 2^t p - 1$. For vertices a and $(n+1-a)$, condition a) of Theorem 4.2.4 is satisfied with $2\sigma_j = 1 + (-1)^j$, by Lemma 3.3.7.

The eigenvalues of the path P_n belong to the cyclotomic field $\mathbb{Q}(\zeta_{2m})$, where $m = n+1$ and ζ_{2m} is a $2m$th primitive root of unity. More precisely, the eigenvalues of P_n are

$$\theta_j = 2\cos\left(\frac{j\pi}{m}\right) = \zeta_{2m}^{j} + \zeta_{2m}^{-j} \in \mathbb{Q}(\zeta_{2m}).$$

If $m = 2^t p$, then the *cyclotomic polynomial* is

$$\Phi_{2m}(x) = \sum_{i=0}^{p-1} (-1)^i x^{2^k i}.$$

We will proceed by showing that condition b) of Theorem 4.2.4 holds. If a is a multiple of 2^{t-1}, suppose there is a linear combination of the eigenvalues in Θ_a, satisfying

$$\sum_{j=1}^{n} \ell_j \theta_j = 0,$$

where we make $\ell_j = 0$ if $\theta_j \notin \Theta_a$. By Lemma 3.3.6, θ_j belongs to Θ_a if and only if $2p$ does not divide j.

We define the polynomial $P(x)$ as follows:

$$P(x) = \sum_{j=1}^{n} \ell_j x^j + \sum_{j=n+2}^{2n+1} \ell_{2n+2-j} x^j$$

We see that ζ_{2m} is a root of $P(x)$ and, since $\Phi_{2m}(x)$ is the minimal polynomial of ζ_{2m}, we see that $\Phi_{2m}(x)$ divides $P(x)$.

Let $Q(x)$ be the following polynomial:

$$Q(x) = \sum_{j=1}^{2^t} \ell_j x^j + \sum_{j=2^t+1}^{2^t p-1} (\ell_j + \ell_{j-2^t}) x^j + \ell_{2^t(p-1)} x^{2^t p} + \sum_{j=1}^{2^t-1} (\ell_{2^t p-j} + \ell_{2^t(p-1)+j} - \ell_j) x^{2^t p+j}. \quad (4.1)$$

For a polynomial $p(x)$, we denote by $[x^t]p(x)$ the coefficient of x^t in $p(x)$. Consider $[x^k]\Phi_{2m}(x)Q(x)$. It is easy to see that $[x^k]\Phi_{2m}(x)Q(x) = [x^k]P(x)$ for $k = 0, \ldots, 2^t(p+1)-1$. Since the degree of $Q(x)$ is $2^t(p+1)-1$, we may conclude that $Q(x)$ is the unique polynomial of degree $2^t(p+1)-1$ such that

$$[x^k]\Phi_{2m}(x)Q(x) = [x^k]P(x)$$

for $k = 0, \ldots, 2^t(p+1)-1$. In particular, the quotient $P(x)/\Phi_{2m}(x)$ is a polynomial of degree $2^t(p+1)-1$ such that (4.3) holds, therefore

$$P(x) = \Phi_{2m}(x)Q(x).$$

From the coefficients of x^k for $k > 2^t(p+1)-1$, it follows that, for $j = 2, 4, \ldots, 2^{t-1}-2$, and $i = 1, \ldots, (p-1)/2$,

$$\begin{aligned} \ell_j - \ell_{2^t p-j} &= (-1)^i (\ell_{i2^t \pm j} - \ell_{(p-i)2^t \mp j}), \\ \ell_{i2^{t-1}} - \ell_{(p-i)2^{t-1}} &= 0. \end{aligned}$$

Recall that $\ell_{2kp} = 0$ for any integer k.

Given $j \in \{2, 4, \ldots, 2^{t-1}-2\}$, note that $j \not\equiv 0 \pmod p$, and since $2^t \not\equiv 0 \pmod p$, there is $i \in \mathbb{Z}_p$ such that $i2^t \equiv j \pmod p$. If $1 \le i \le (p-1)/2$, then $\ell_{i2^t-j} = \ell_{(p-i)2^t+j} = 0$, and if $(p-1)/2+1 \le i \le p-1$, then $\ell_{i2^t+j} = \ell_{(p-i)2^t-j} = 0$. In either case, it follows that $\ell_j - \ell_{2^t p-j} = 0$. Therefore $\ell_j = \ell_{2^t p-j}$ for all even j.

Thus, we see that

$$\sum_{\theta_r \in \Theta_a} \ell_j \zeta_j = \sum_{j \text{ even}} \ell_r \equiv \ell_{2^{t-1}p} \equiv 0 \pmod 2,$$

which concludes the proof. □

To complete the characterization, which was recently published in [45], it remains to show that this is the only such family of paths with pretty good state transfer between internal vertices. We begin by presenting the following identity that will be used to apply Theorem 4.2.4. Its derivation is a straightforward application of basic trigonometric identities and is included for completeness.

4.3.2 Lemma. *Let $n = km$, where k is a positive integer and $m > 1$ is an odd integer, and $0 \leq a < k$ be an integer. Then*

$$\sum_{j=0}^{m-1} (-1)^j \cos\left(\frac{(a+jk)\pi}{n}\right) = 0.$$

Proof. Working from the left hand side, we first use the angle sum identity and simplify to obtain

$$\cos\left(\frac{a\pi}{n}\right) \sum_{j=0}^{m-1} (-1)^j \cos\left(\frac{jk\pi}{n}\right) - \sin\left(\frac{a\pi}{n}\right) \sum_{j=0}^{m-1} (-1)^j \sin\left(\frac{jk\pi}{n}\right).$$

We then observe that $(-1)^j \cos(j\theta) = \cos(j(\pi+\theta))$ and $(-1)^j \sin(j\theta) = \sin(j(\pi+\theta))$, hence obtaining

$$\cos\left(\frac{a\pi}{n}\right) \sum_{j=0}^{m-1} \cos\left(\frac{j(k+n)\pi}{n}\right) - \sin\left(\frac{a\pi}{n}\right) \sum_{j=0}^{m-1} \sin\left(\frac{j(k+n)\pi}{n}\right).$$

We can then observe that

$$\begin{aligned}\sum_{j=0}^{m-1} \cos\left(\frac{j(k+n)\pi}{n}\right) + i \sum_{j=0}^{m-1} \sin\left(\frac{j(k+n)\pi}{n}\right) &= \sum_{j=0}^{m-1} \exp\left(\frac{ij(k+n)\pi}{n}\right) \\ &= \frac{\exp\left(\frac{im(k+n)\pi}{n}\right) - 1}{\exp\left(\frac{i(k+n)\pi}{n}\right) - 1} = 0,\end{aligned}$$

as $m(k+n)/n = m+1$ is an even integer. Hence, we have

$$\sum_{j=0}^{m-1} \cos\left(\frac{j(k+n)\pi}{n}\right) = 0, \qquad \sum_{j=0}^{m-1} \sin\left(\frac{j(k+n)\pi}{n}\right) = 0,$$

which completes the proof. □

We now have the tools required to complete the characterization.

4.3.3 Theorem. *There is pretty good state transfer on P_n between vertices a and b if and only if $a + b = n + 1$ and:*

a) $n = 2^t - 1$*, where* t *is a positive integer;*

b) $n = p - 1$*, where* p *is an odd prime; or*

c) $n = 2^t p - 1$*, where* t *is a positive integer and* p *is an odd prime, and* a *is a multiple of* 2^{t-1}*.*

Proof. The sufficiency of the conditions is given by Theorem 4.2.2 and Theorem 4.3.1. It remains to show that the conditions are necessary. The necessity of the condition that $a + b = n + 1$ follows from Lemma 3.2.6 and 3.3.7. Henceforth, we need only consider the possibility of pretty good state transfer between vertices a and $n + 1 - a$. We note that if $a = (n + 1)/2$, we would instead be considering almost periodicity at a rather than pretty good state transfer, and hence we will exclude this case in what follows.

Suppose that there is pretty good state transfer on P_n between vertices a and $n+1-a$. We first observe that every integer n can be written in the form $2^t r - 1$, where t is a nonnegative integer and r is a positive odd integer. We consider multiple cases based on the values of t and r.

Case 1: $t > 0$ **and** r **is an odd composite number**

First, suppose r has no prime factor p such that p divides $2^t r / \gcd(a, 2^t r)$. It follows that $r \mid a$. Moreover, since a and $n + 1 - a$ are distinct vertices, then $a \neq 2^{t-1} r$. Hence, we have that $t \geq 2$ and 4 divides $2^t r / \gcd(a, 2^t r)$, so by Lemma 3.3.6, if k is not a multiple of 4, then $\theta_k \in \Theta_a$. Now, consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k \equiv 1, 2^t + 2 \pmod{2^{t+1}}; \\ -1, & \text{if } k \equiv 2, 2^t + 1 \pmod{2^{t+1}}; \\ 0, & \text{otherwise.} \end{cases}$$

For $c \in \{1, 2\}$, we have

$$\sum_{i=0}^{r-1} (-1)^i \theta_{c+i2^t} = \sum_{i=0}^{r-1} (-1)^i \cos\left(\frac{(c + i2^t)\pi}{n + 1}\right) = 0$$

by Lemma 4.3.2. Hence we see that

$$\sum_k \ell_k \theta_k = 0, \tag{4.2}$$

$$\sum_k \ell_k \zeta_k \text{ is odd}, \tag{4.3}$$

$$\sum_k \ell_k = 0, \tag{4.4}$$

so by Theorem 4.2.4, we cannot have pretty good state transfer between a and $n+1-a$.

Therefore, we can now assume r has a prime factor p such that p divides $2^t r/\gcd(a, 2^t r)$. By Lemma 3.3.6, if k is not a multiple of p, then $\theta_k \in \Theta_a$. Now, consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k \equiv 1, 2^t p + 2 \pmod{2^{t+1}p}; \\ -1, & \text{if } k \equiv 2, 2^t p + 1 \pmod{2^{t+1}p}; \\ 0, & \text{otherwise.} \end{cases}$$

For $c \in \{1, 2\}$, we have

$$\sum_{i=0}^{r/p-1} (-1)^i \theta_{c+i2^t p} = \sum_{i=0}^{r/p-1} (-1)^i \cos\left(\frac{(c+i2^t p)\pi}{n+1}\right) = 0$$

by Lemma 4.3.2. So we see that (4.2), (4.3), and (4.4) again hold, so by Theorem 4.2.4, we cannot have pretty good state transfer between a and $n+1-a$.

Case 2: $t = 0$ and r is an odd composite number

There exists a prime factor p of r such that p divides $r/\gcd(a, r)$, as otherwise r divides a, contradicting that $a < r = n+1$. By Lemma 3.3.6, if k is not a multiple of p, then $\theta_k \in \Theta_a$. Now, consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k \equiv 1, p+2 \pmod{2p}; \\ -1, & \text{if } k \equiv 2, p+1 \pmod{2p}; \\ 0, & \text{otherwise.} \end{cases}$$

For $c \in \{1, 2\}$, we have

$$\sum_{i=0}^{r/p-1} (-1)^i \theta_{c+ip} = \sum_{i=0}^{r/p-1} (-1)^i \cos\left(\frac{(c+ip)\pi}{n+1}\right) = 0$$

by Lemma 4.3.2. Hence we see that (4.2), (4.3), and (4.4) again hold, so by Theorem 4.2.4, we cannot have pretty good state transfer between a and $n+1-a$.

Case 3: $t > 0$ **and** $r = p$ **is an odd prime number**

Suppose a is not a multiple of 2^{t-1}. Then again by Lemma 3.3.6, if k is not a multiple of 4, then $\theta_k \in \Theta_a$. It follows as in the first case that we cannot have pretty good state transfer between a and $n+1-a$.

Hence we have shown the stated conditions are necessary, completing the proof. □

4.4 Laplacian Model

We now consider pretty good state transfer between internal vertices of paths with respect to the Laplacian. The procedure is similar to that for the adjacency matrix. The eigenvalues of $L(P_n)$ are $\theta_0 := 0$ with the all 1s eigenvector, and $\theta_k := 2 + 2\cos(\pi k/n)$, $1 \leq k < n$, with corresponding eigenvector v^k given by

$$v_a^k = (-1)^a(\sin((a-1)\pi k/n) + \sin(a\pi k/n)).$$

We begin by determining the eigenvalue support of a vertex.

4.4.1 Lemma. *The eigenvalue support of vertex a of the graph P_n with respect to the Laplacian is given by*

$$\Theta_a = \{0\} \cup \{\theta_k : 2n \nmid (2a-1)k\}.$$

Proof. We first observe for the path that $E_k \mathbf{e}_a = 0$ if and only if $v_a^k = 0$. Let us consider the value of v_a^k. Using a sum identity, we obtain

$$v_a^k = 2\sin((2a-1)\pi k/2n)\cos(\pi k/2n).$$

Notice that since $1 \leq k < n$, we have $\cos(\pi k/2n) > 0$. Hence $v_a^k = 0$ if and only if $\sin((2a-1)\pi k/2n) = 0$, which is precisely when $2n \mid (2a-1)k$. The result follows. □

We will also make use of the following identity, the derivation of which is a straightforward application of basic trigonometric identities and geometric series and is included for completeness.

4.4.2 Lemma. *Let $n = 4k+2$, where k is a positive integer. Then*

$$2\sum_{j=0}^{k-1}\left(2+2\cos\left(\frac{(2+4j)\pi}{n}\right)\right) = n.$$

Proof. We first use the fact that $2\cos x = e^{ix} + e^{-ix}$ to obtain

$$2\sum_{j=0}^{k-1}\cos\left(\frac{(2+4j)\pi}{n}\right) = \sum_{j=0}^{k-1}\left(e^{\frac{i(2+4j)\pi}{n}} + e^{\frac{-i(2+4j)\pi}{n}}\right).$$

Using the formula for geometric series, we then have

$$2\sum_{j=0}^{k-1}\cos\left(\frac{(2+4j)\pi}{n}\right) = \left(e^{\frac{2\pi i}{n}}\right)\frac{1-\left(e^{\frac{4\pi i}{n}}\right)^k}{1-e^{\frac{4\pi i}{n}}} + \left(e^{\frac{-2\pi i}{n}}\right)\frac{1-\left(e^{\frac{-4\pi i}{n}}\right)^k}{1-e^{\frac{-4\pi i}{n}}}.$$

For the last term, we multiply numerator and denominator by $e^{\frac{4\pi i}{n}}$ and hence obtain

$$2\sum_{j=0}^{k-1}\cos\left(\frac{(2+4j)\pi}{n}\right) = \left(e^{\frac{2\pi i}{n}}\right)\frac{1-\left(e^{\frac{4\pi i}{n}}\right)^k}{1-e^{\frac{4\pi i}{n}}} - \left(e^{\frac{2\pi i}{n}}\right)\frac{1-\left(e^{\frac{-4\pi i}{n}}\right)^k}{1-e^{\frac{4\pi i}{n}}}.$$

Simplifying, we obtain

$$2\sum_{j=0}^{k-1}\cos\left(\frac{(2+4j)\pi}{n}\right) = \frac{-e^{\frac{(4k+2)\pi i}{4k+2}} + e^{\frac{-(4k+2)\pi i}{4k+2}}e^{\frac{4\pi i}{n}}}{1-e^{\frac{4\pi i}{n}}} = \frac{1-e^{\frac{4\pi i}{n}}}{1-e^{\frac{4\pi i}{n}}} = 1.$$

Thus, evaluating our original expression, we obtain

$$2\sum_{j=0}^{k-1}\left(2+2\cos\left(\frac{(2+4j)\pi}{n}\right)\right) = 4k+2 = n,$$

as desired. □

We now have the tools we need to demonstrate that there are no additional examples of pretty good state transfer on paths with respect to the Laplacian when considering internal vertices.

4.4.3 Theorem. *There is pretty good state transfer on P_n between vertices a and b with respect to the Laplacian if and only if $a + b = n + 1$ and n is a power of 2.*

Proof. The sufficiency of the conditions is given by Theorem 4.2.3. It remains to show that the conditions are necessary. The necessity of the condition that $a+b = n+1$ follows from Lemma 3.2.6 and 3.3.7. Henceforth, we need only consider the possibility of pretty good state transfer between vertices a and $n + 1 - a$. We again note that if $a = (n + 1)/2$, we would instead be considering almost periodicity at a rather than pretty good state transfer, and hence we will exclude this case in what follows.

Suppose n is not a power of 2 and that there is pretty good state transfer on P_n between vertices a and $n + 1 - a$. We first observe that every integer n can be written in the form $2^t r$, where t is a nonnegative integer and r is a positive odd integer greater than 1. We consider multiple cases based on the values of t and r.

Case 1: $t > 1$

Since $2a-1$ is odd, it follows that 4 divides $2^{t+1}r/\gcd(2a-1, 2^{t+1}r)$. By Lemma 4.4.1, if k is not a multiple of 4, then $\theta_k \in \Theta_a$. Now consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k \equiv 1, 2^t + 2 \pmod{2^{t+1}}; \\ -1, & \text{if } k \equiv 2, 2^t + 1 \pmod{2^{t+1}}; \\ 0, & \text{otherwise.} \end{cases}$$

For $c \in \{1, 2\}$, we have

$$\sum_{j=0}^{r-1} (-1)^j \theta_{c+j2^t} = \sum_{i=0}^{r-1} (-1)^j (2 + 2\cos\left(\frac{(c + j2^t)\pi}{n}\right) = 2$$

by Lemma 4.3.2. So we see that (4.2), (4.3), and (4.4) hold, so by Theorem 4.2.4, we cannot have pretty good state transfer between a and $n + 1 - a$.

Case 2: $t = 1$

Since $2a - 1$ is odd, it follows that 4 divides $4r/\gcd(2a - 1, 4r)$. By Lemma 4.4.1, if k is not a multiple of 4, then $\theta_k \in \Theta_a$. Now consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 2, & \text{if } k \equiv 2 \pmod 4; \\ -r, & \text{if } k = r; \\ 1, & \text{if } k = 0; \\ 0, & \text{otherwise.} \end{cases}$$

We have

$$2\sum_{j=0}^{\frac{r-3}{2}}\left(2+2\cos\left(\frac{(2+4j)\pi}{n}\right)\right)=n.$$

by Lemma 4.4.2 and $\theta_r = 2$. So we see that (4.2), (4.3), and (4.4) again hold, so by Theorem 4.2.4, we cannot have pretty good state transfer between a and $n+1-a$.

Case 3: $t = 0$ and r is an odd composite number

There exists a prime factor p of r such that p divides $2r/\gcd(2a-1, 2r)$, as otherwise r divides $2a-1$ which implies $a = (r+1)/2$, and as a is the middle vertex of the path, we do not consider it for pretty good state transfer. By Lemma 4.4.1, if k is not a multiple of p, then $\theta_k \in \Theta_a$. Now, consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k \equiv 1, p+2 \pmod{2p}; \\ -1, & \text{if } k \equiv 2, p+1 \pmod{2p}; \\ 0, & \text{otherwise.} \end{cases}$$

For $c \in \{1, 2\}$, we have

$$\sum_{j=0}^{r/p-1}(-1)^j\theta_{c+jp} = \sum_{i=0}^{r/p-1}(-1)^j(2+2\cos\left(\frac{(c+jp)\pi}{n}\right) = 2$$

by Lemma 4.3.2. So we see that (4.2), (4.3), and (4.4) again hold, so by Theorem 4.2.4, we cannot have pretty good state transfer between a and $n+1-a$.

Case 4: $t = 0$ and r is an odd prime

If r is an odd prime, then there is no eigenvalue not in the eigenvalue support of a; such an eigenvalue would require $2r$ to divide $(2a-1)k$. Since r is prime and $k < r$, we would need r to divide $2a-1$, and since $a \leq r$, it implies $a = (r+1)/2$. But as a is the middle vertex of the path, we do not consider it for pretty good state transfer. Hence, every eigenvalue is in the eigenvalue support of a, and so if there is pretty good state transfer between vertices a and $n+1-a$, then there must also be pretty good state transfer between vertices 1 and n, but this contradicts Theorem 4.2.3. Hence, we cannot have pretty good state transfer between a and $n+1-a$.

Hence we have shown the necessity of the stated conditions, completing the proof. □

4.5 Future Directions

One of the major open problems regarding this research stems from the fact that Kronecker's Theorem provides us with a non-constructive proof technique to demonstrate pretty good state transfer. As such, we are, for the most part, unable to say anything about the length of time it takes to achieve state transfer with a given precision. Coutinho and Godsil [20] provide a brief discussion in the case of P_4, showing that the approximation using $\tau = 305\pi \approx 958$ is accurate to five decimal places (i.e. 99.999% state transfer), illustrating that the length of time required is typically very large.

A question that provides further motivation to considering pretty good state transfer on internal vertices of paths is the minimum number of edges required to achieve pretty good state transfer of distance d, which would minimize the cost of a quantum communication channel. Pretty good state transfer on internal vertices of paths provides some bounds on this question. For example, if we wish to achieve state transfer between vertices at distance 16, this cannot be achieved on P_{17}, but can be achieved between vertices 2 and 18 of P_{19}, compared to using vertices 3 and 19 of P_{21} if we only limit ourselves to paths with pretty good state transfer between the end vertices. The question remains open, as other graphs may provide pretty good state transfer using fewer edges, i.e. we would still need to consider whether pretty good state transfer at distance 16 can be achieved with 17 edges.

Therefore, another area of interest would be to expand the graphs considered from paths to trees to provide additional sparse examples towards settling the question above. Some results for pretty good state transfer with respect to the adjacency matrix were provided by Fan and Godsil [24] for the case of double stars.

4.5.1 Theorem. *[24] There is pretty good state transfer in the double star $S_{k,\ell}$:*

a) For $k = 2, \ell \geq 3$, between the two leaves incident with the degree three vertex.

b) For $k, \ell \geq 3$, between the internal vertices if and only if $k = \ell$ and $4k + 1$ is a perfect square.

Chapter 5

State Transfer of Multiple Qubits

Given that the length of time required to achieve pretty good state transfer is typically very large, if we wish to transfer multiple states, it would be largely impractical to do so one state at a time. One possible alternative is to set up multiple spin chains and run them simultaneously, though this may be cost prohibitive depending on the number of qubits involved. An alternative is to send a state consisting of multiple qubits through the same channel, which we consider in this chapter. We will discuss two special cases of the general problem of transferring multi-qubit states: transfer to a symmetric state and fractional revival.

5.1 Transfer to a Symmetric State

In 2014, Sousa and Omar [43] extended the definition of pretty good state transfer to arbitrary multi-qubit states. For the single excitation case, they say there is *pretty good state transfer* on P_n of the m-qubit state $\mathbf{v}$, given by

$$\alpha\mathbf{0} + \sum_{j=1}^{m} \beta_j \mathbf{e}_j, \quad |\alpha|^2 + \sum_{j=1}^{m} |\beta_j|^2 = 1,$$

from qubits 1 to m to qubits $n-m+1$ to n if for every $\epsilon > 0$, there exist a time $\tau_\epsilon \in \mathbb{R}$ and complex numbers $(\gamma_j)_\epsilon$, where $|(\gamma_j)_\epsilon| = 1$, such that

$$||U(\tau_\epsilon)\mathbf{e}_j - (\gamma_j)_\epsilon \mathbf{e}_{n+1-j}|| < \epsilon,$$

for $1 \leq j \leq m$. It follows similarly to the single vertex case (Proposition 4.0.1) that assuming γ_j is fixed is equivalent.

The above definition appears to be more strict than required, as a multiple qubit state need not involve all of the first m qubits of the chain. Additionally, their definition of pretty good state transfer is restricted to the case when the graph is a path. Hence, we say a graph X has *pretty good state transfer* between distinct states $\mathbf{v}$ and $\mathbf{w}$ if, for every $\epsilon > 0$, there exist a time $\tau_\epsilon \in \mathbb{R}$ and a complex number γ_ϵ, where $|\gamma_\epsilon| = 1$, such that

$$||U(\tau_\epsilon)\mathbf{v} - \gamma_\epsilon \mathbf{w}|| < \epsilon.$$

If the above is satisfied for $\epsilon = 0$, then we say there is perfect state transfer of $\mathbf{v}$. We again observe following Proposition 4.0.1 that it is equivalent to consider a fixed γ. If we allow $\mathbf{v} = \mathbf{w}$, then we would be considering whether the state $\mathbf{v}$ is *almost periodic*, and would be interested if there are times $\tau_\epsilon \neq 0$ where the above inequality holds. Corollary 4.1.2 guarantees the existence of such times.

We will restrict our consideration to single-excitation states, that is, we will require $\mathbf{v}$ and $\mathbf{w}$ to be in the form

$$\sum_{a \in V(X)} \beta_a \mathbf{e}_a, \qquad \sum_{a \in V(X)} \beta_a^2 = 1.$$

Such a restriction is motivated by our simplification of considering the $n \times n$-dimensional subspace of states spanned by single vertex states rather than the entire $2^n \times 2^n$ state space.

Of course, one could find many instances of perfect state transfer between arbitrary pairs of states by choosing $\mathbf{v}$ at will, choosing an arbitrary τ, and then letting $\mathbf{w} = U(\tau)\mathbf{v}$. Hence, motivated by the symmetry exhibited by the path, we are primarily interested in pretty good state transfer in X between states $\mathbf{v}$ and $\mathbf{v}^\sigma$, where σ is an automorphism of X and $\mathbf{v}^\sigma$ is given by

$$\mathbf{v}^\sigma = \sum_{x \in V(X)} \beta_x \mathbf{e}_{\sigma(x)}, \qquad \mathbf{v} = \sum_{x \in V(X)} \beta_x \mathbf{e}_x.$$

We will consider this problem in what follows.

Sousa and Omar [43] demonstrated a class of examples exhibiting pretty good state transfer to a symmetric state by applying the following theorem due to Cameron et al. [9]. We first need to present the following definitions. A square matrix is said to be *monomial*, and denoted $\widetilde{P}_\phi$, if it is the product of the permutation matrix P_ϕ and some complex diagonal matrix D (which is suppressed in the notation). Then, two *Hermitian graphs* X

and Y, that is, graphs whose adjacency matrices are Hermitian, are said to be *switching isomorphic* if there is a monomial matrix $\widetilde{P}_\phi$ such that $A(Y) = \widetilde{P}_\phi^\dagger A(X)\widetilde{P}_\phi$. Notice that if $D = I$, then X and Y are isomorphic. The switching automorphism group of a graph X is defined to be the group of monomial matrices that commute with $A(X)$, and is denoted $\mathsf{SwAut}(X)$.

5.1.1 Theorem. *[9] Let X be an n-vertex graph with pretty good state transfer from vertex a to vertex $\phi(a)$, for some switching automorphism $\widetilde{P}_\phi \in \mathsf{SwAut}(X)$. Suppose that $A(X)$ and $\widetilde{P}_\phi$ share a set $\{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$ of orthonormal eigenvectors which satisfies $\mathbf{e}_a^T\mathbf{z}_k \neq 0$ for $1 \leq k \leq n$. Then, for each $\epsilon > 0$, there is a time $t \in \mathbb{R}$ where*

$$||e^{-itA(X)} - \gamma\widetilde{P}_\phi|| \leq \epsilon,$$

for some $\gamma \in \mathbb{C}$, $|\gamma| = 1$.

5.1.2 Corollary. *[43] If the multi-qubit input state $\mathbf{v}$ is restricted to the single-excitation manifold, then there is pretty good state transfer of $\mathbf{v}$ on P_n to the mirror image if we have $n = p-1, 2p-1$, or $2^k - 1$, where p is a prime and $k \in \mathbb{N}$.*

Proof. Suppose $n = p-1, 2p-1$, or $2^k - 1$. Then by Theorem 5.1.1, for each $\epsilon > 0$, there is a time $t \in \mathbb{R}$ where

$$||U(t) - \gamma\widetilde{P}_\phi|| \leq \epsilon,$$

for some $\gamma \in \mathbb{C}$, $|\gamma| = 1$. Since $||\mathbf{v}|| = 1$, we have

$$\epsilon \geq ||U(t) - \gamma\widetilde{P}_\phi||\ ||\mathbf{v}|| = ||U(t)\mathbf{v} - \gamma\widetilde{P}_\phi\mathbf{v}|| = ||U(t)\mathbf{v} - \gamma\mathbf{v}^\sigma||$$

as desired. □

Sousa and Omar [43] claimed the preceding result gave both necessary and sufficient conditions, however, they only provide a proof that the conditions on n are sufficient. Under our more general definition of pretty good state transfer, the conditions are not necessary, as demonstrated by the following example.

5.1.3 Example. We can verify there is pretty good state transfer on P_{11} between states $\mathbf{v} = \frac{1}{\sqrt{2}}(\mathbf{e}_1 + \mathbf{e}_3)$ and $\mathbf{v}^\sigma = \frac{1}{\sqrt{2}}(\mathbf{e}_{11} + \mathbf{e}_9)$. We first demonstrate that $\theta_6 = 0 \notin \Theta_\mathbf{v}$. We have that

$$(E_6\mathbf{v})_x = \frac{1}{\sqrt{2}}((E_6)_{x,1} + (E_6)_{x,3}) = \frac{1}{\sqrt{2}}\left(\frac{1}{6}\sin\left(\frac{\pi x}{2}\right)\sin\left(\frac{\pi}{2}\right) + \frac{1}{6}\sin\left(\frac{\pi x}{2}\right)\sin\left(\frac{3\pi}{2}\right)\right) = 0,$$

and so $E_6\mathbf{v} = \mathbf{0}$ as claimed.

Now, by definition, we wish to show

$$\|U(\tau)\mathbf{v} - \gamma\mathbf{v}^\sigma\| < \epsilon,$$

which, using spectral decomposition, is equivalent to

$$\left\| \left(\sum_{\theta_j \in \Theta_\mathbf{v}} \exp(i\tau\theta_j)(E_j)\mathbf{v} \right) - \gamma\mathbf{v}^\sigma \right\| < \epsilon.$$

We observe that $E_r\mathbf{v} = E_r\mathbf{v}^\sigma$ when r is odd and $E_r\mathbf{v} = -E_r\mathbf{v}^\sigma$ when r is even (i.e. by linearity), and letting $\gamma = \exp(i\delta)$, we have

$$\left\| \sum_{\theta_j \in \Theta_\mathbf{v}} (\exp(i\tau\theta_j) - (-1)^{j+1}\exp(i\delta))E_j\mathbf{v} \right\| < \epsilon,$$

from which it follows that we desire

$$|\tau\theta_j - (\delta + \sigma_r\pi)| < \epsilon' \pmod{2\pi}, \qquad (r : \theta_r \in \Theta_\mathbf{v}),$$

where σ_r is even if r is odd and odd if r is even.

If we let $\delta = 0$, then the inequalities corresponding to θ_j and θ_{11-j} only differ by a factor of -1, so it suffices to consider the system

$$\left| \frac{\sqrt{6}+\sqrt{2}}{2}\tau \right| < \epsilon \pmod{2\pi},$$

$$\left| \sqrt{3}\tau + \pi \right| < \epsilon \pmod{2\pi},$$

$$\left| \sqrt{2}\tau \right| < \epsilon \pmod{2\pi},$$

$$|\tau + \pi| < \epsilon \pmod{2\pi},$$

$$\left| \frac{\sqrt{6}-\sqrt{2}}{2}\tau \right| < \epsilon \pmod{2\pi}.$$

In order to apply Kronecker's Theorem, we need to show that for every integer solution to the equation

$$\frac{\sqrt{6}+\sqrt{2}}{2}\ell_1 + \sqrt{3}\ell_2 + \sqrt{2}\ell_3 + \ell_4 + \frac{\sqrt{6}-\sqrt{2}}{2}\ell_5 = 0,$$

we have

$$0(\ell_1 + \ell_3 + \ell_5) + \pi(\ell_2 + \ell_4) \equiv 0 \pmod{2\pi}.$$

Since the only integer solutions are of the form $\ell_1 = -\ell_3 = -\ell_5$, $\ell_2 = \ell_4 = 0$, the above equation is satisfied. Hence we can apply Kronecker's Theorem, which verifies that we have pretty good state transfer between states $\mathbf{v} = \frac{1}{\sqrt{2}}(\mathbf{e}_1 + \mathbf{e}_3)$ and $\mathbf{v}^\sigma = \frac{1}{\sqrt{2}}(\mathbf{e}_{11} + \mathbf{e}_9)$. $\diamondsuit$

In 2018, Vieira and Rigolin [46] summarized the previous work considering quantum state transmission into three topics: (a) the transfer of a single excitation or an arbitrary qubit from Alice to Bob, (b) the creation of a highly entangled state between Alice and Bob, and (c) the transfer of multiple excitations or multiple qubit states from Alice to Bob. In each of these problems, the main consideration is transfer on a path, so for (a), the transfer is typically studied between vertices 1 and n; for (b), the transfer is typically studied between vertices 1 and 2 and 1 and n; and for (c), the transfer is typically studied between vertices 1 and 2 and $n-1$ and n. In their paper, the authors focus on the transfer of maximally entangled two-qubit states, or Bell states, and investigate the transmission of the pairwise entanglement between Alice's starting state and Bob's ending state. They vary the coupling constants (edge weights) between the vertices and numerically assess the greatest pairwise entanglement transmission. They also vary the path by adding an additional leaf at each end, extending slightly beyond the 1-dimensional case. The authors claim that this modification is crucial to have almost perfect transmission of a Bell state without modulation or external fields, but this appears to contradict Corollary 5.1.2.

We proceed by examining paths of certain lengths and states of a particular form, and characterizing pretty good state transfer of multiple qubit states in terms of the eigenvalue support of the states. Our approach is analogous to the proofs of Theorem 4.3.1 and Theorem 4.3.3. The *eigenvalue support* of a state $\mathbf{v}$ is the set of eigenvalues θ such that $E_\theta \mathbf{v} \neq 0$, and is denoted by $\Theta_{\mathbf{v}}$. We begin by generalizing the notion of strong cospectrality to multiple qubit states. We say that two states $\mathbf{v}$ and $\mathbf{w}$ of X are *cospectral* if for each idempotent E_r in the spectral decomposition of X, we have $\mathbf{v}^\dagger E_r \mathbf{v} = \mathbf{w}^\dagger E_r \mathbf{w}$, *parallel* if for each eigenvalue θ_r, the vectors $E_r\mathbf{v}$ and $E_r\mathbf{w}$ are parallel, and *strongly cospectral* if for each eigenvalue θ_r, there exists a γ_r such that $|\gamma_r| = 1$ and $E_r\mathbf{v} = \gamma_r E_r \mathbf{w}$ (Note that unlike in the case of a single vertex, we cannot assume the states are real, which allowed us to simplify γ_r to ± 1.). Recalling Lemma 2.3.3, we verify that these generalizations match our intuition.

5.1.4 Lemma. *Two states* $\mathbf{v}$ *and* $\mathbf{w}$ *in* X *are strongly cospectral if and only if they are parallel and cospectral.*

Proof. Suppose states $\mathbf{v}$ and $\mathbf{w}$ are strongly cospectral. It immediately follows from the definition that $\mathbf{v}$ and $\mathbf{w}$ are parallel. We verify that $\mathbf{v}$ and $\mathbf{w}$ are cospectral by observing

$$\mathbf{v}^\dagger E_r \mathbf{v} = \gamma_r \mathbf{v}^\dagger E_r \mathbf{w} = \gamma_r \overline{\gamma}_r \mathbf{w}^\dagger E_r \mathbf{w} = \mathbf{w}^\dagger E_r \mathbf{w}$$

using the fact that the idempotents are symmetric.

Conversely, suppose $\mathbf{v}$ and $\mathbf{w}$ are parallel and cospectral. It follows that

$$\mathbf{w}^\dagger E_r \mathbf{v} = c\mathbf{w}^\dagger E_r \mathbf{w} = c\mathbf{v}^\dagger E_r \mathbf{v} = c\overline{c}\mathbf{w}^\dagger E_r \mathbf{v} = |c|^2 \mathbf{w}^\dagger E_r \mathbf{v}$$

again using the fact that idempotents are symmetric. Hence it follows that if $\mathbf{v}^\dagger E_r \mathbf{w}$ is nonzero, then $|c|^2 = 1$, so $c = \gamma_r$, $|\gamma_r| = 1$ as required.

Now consider the situation when $\mathbf{v}^\dagger E_r \mathbf{w} = 0$. Since $\mathbf{v}$ and $\mathbf{w}$ are parallel, it follows that $\mathbf{v}^\dagger E_r \mathbf{v} = \mathbf{w}^\dagger E_r \mathbf{w} = 0$. We then observe that

$$\|E_r \mathbf{v}\|^2 = \mathbf{v}^\dagger E_r^\dagger E_r \mathbf{v} = \mathbf{v}^\dagger E_r \mathbf{v} = 0,$$

using the fact that E_r is symmetric and idempotent. Similarly, $\|E_r \mathbf{w}\|^2 = 0$. Hence $E_r \mathbf{v} = E_r \mathbf{w} = 0$ as required. □

We continue by verifying that strong cospectrality is a requirement for pretty good state transfer in this more general case.

5.1.5 Lemma. *Let* X *be a graph, and let* $\mathbf{v}, \mathbf{w}$ *be states of* X*. If there is pretty good state transfer from* $\mathbf{v}$ *to* $\mathbf{w}$*, then* $\mathbf{v}$ *and* $\mathbf{w}$ *are strongly cospectral.*

Proof. By definition, if we have pretty good state transfer from $\mathbf{v}$ to $\mathbf{w}$ in X, then there exists a sequence of times $\{t_k\}$ such that

$$\lim_{k\to\infty} |\mathbf{w}^\dagger U(t_k)\mathbf{v}| = 1.$$

We calculate the following:

$$\begin{aligned}
1 &= \lim_{k\to\infty} |\mathbf{w}^\dagger U(t_k)\mathbf{v}| \\
&\le \sum_\theta |\mathbf{w}^\dagger E_\theta \mathbf{v}| \\
&\le \sum_\theta \sqrt{\mathbf{v}^\dagger E_\theta \mathbf{v}}\sqrt{\mathbf{w}^\dagger E_\theta \mathbf{w}} \\
&\le \sqrt{\sum_\theta \mathbf{v}^\dagger E_\theta \mathbf{v} \sum_\theta \mathbf{w}^\dagger E_\theta \mathbf{w}} \\
&= 1.
\end{aligned}$$

The first inequality is an application of the triangle inequality. The second and third inequalities are applications of Cauchy-Schwarz, where we take $u = E_\theta \mathbf{v}$ and $v = E_\theta \mathbf{w}$ and $u = (\sqrt{\mathbf{v}^\dagger E_\theta \mathbf{v}})_\theta$ and $v = (\sqrt{\mathbf{w}^\dagger E_\theta \mathbf{w}})_\theta$ respectively. The last inequality follows from the spectral decomposition and the definition of $\mathbf{v}, \mathbf{w}$.

Therefore, all inequalities must hold with equality. In particular, the second inequality implies $\mathbf{v}$ and $\mathbf{w}$ are parallel, and the third inequality implies $\mathbf{v}$ and $\mathbf{w}$ are cospectral, which completes the proof. □

Having defined strong cospectrality for multiple qubit states and demonstrated that is is a necessary condition for pretty good state transfer in general, we now restrict our attention to pretty good state transfer on paths between $\mathbf{v}$ and $\mathbf{v}^\sigma$. We first verify the following.

5.1.6 Lemma. *Let $\mathbf{v}$ be a state of a path P_n. Then $\mathbf{v}$ and $\mathbf{v}^\sigma$ are strongly cospectral. Moreover, $E_r\mathbf{v} = (-1)^{r+1}E_r\mathbf{v}^\sigma$.*

Proof. For a given r, we apply Lemma 3.3.7 to obtain

$$\begin{aligned}
E_r\mathbf{v} &= E_r \sum_{a\in V(P_n)} \beta_a \mathbf{e}_a \\
&= \sum_{a\in V(X)} \beta_a E_r \mathbf{e}_a \\
&= \sum_{a\in V(P_n)} \beta_a (-1)^{r+1} E_r \mathbf{e}_{n+1-a}
\end{aligned}$$

$$
\begin{aligned}
&= (-1)^{r+1} E_r \sum_{a \in V(P_n)} \beta_a \mathbf{e}_{n+1-a} \\
&= (-1)^{r+1} E_r \mathbf{v}^\sigma,
\end{aligned}
$$

as desired. □

We now generalize Theorem 4.2.4 to this case.

5.1.7 Theorem. *Let $\mathbf{v}$ be a state of a path P_n, and let $\zeta_j = (1 + (-1)^j)/2$. Then there is pretty good state transfer between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if and only if for every set of integers $\{\ell_j\}$ such that*

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j \theta_j = 0 \quad \textit{and} \quad \sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j \zeta_j \ \textit{is odd,}$$

then

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j \neq 0.$$

Proof. First suppose the condition on the sets of integers $\{\ell_j\}$ is satisfied. We consider the system of inequalities

$$|\theta_j \tau - (\delta + \zeta_j \pi)| < \epsilon \pmod{2\pi}, \qquad (\theta_j \in \Theta_{\mathbf{v}}).$$

Let $\{\ell_j\}$ be a set of integers such that

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j \theta_j = 0.$$

Then we desire

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j (\delta + \zeta_j \pi) \equiv 0 \pmod{2\pi}. \tag{†}$$

We need to show that there exists a δ such that the above equation is true for all sets $\{\ell_j\}$. If $\sum \ell_j \zeta_j$ is even for every set of integers $\{\ell_j\}$, then we may choose $\delta = 0$. Otherwise, suppose for some set of integers $\{\ell_j\}$ that $\sum \ell_j \zeta_j$ is odd, in which case $\alpha := \sum \ell_j \neq 0$, and let δ be such that the above equation is satisfied for this set. Suppose $\{\ell'_j\}$ is also a set of integers such that

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell'_j \theta_j = 0.$$

Define $\alpha' = \sum \ell'_j$, and let 2^r be the largest power of 2 that divides α, 2^s be the largest power of 2 that divides α', and $t = \min\{r, s\}$. Take $\delta = \pi 2^{-r}$. Then we construct the set of integers $\gamma_j = 2^{-t}(\alpha'\ell_j - \alpha\ell'_j)$. It is a straightforward calculation that $\sum \gamma_j \theta_j = 0$ and $\sum \gamma_j = 0$. Now consider the expression

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \gamma_j \zeta_j = \sum_{\theta_j \in \Theta_{\mathbf{v}}} 2^{-t}(\alpha'\ell_j - \alpha\ell'_j)\zeta_j = \left(2^{-t}\alpha'\right)\left(\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j \zeta_j\right) - \left(2^{-t}\alpha\right)\left(\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell'_j \zeta_j\right).$$

We observe that $\sum \gamma_j \zeta_j$ is even, as otherwise we have a contradiction to our hypothesis, $\sum \ell_j \zeta_j$ is odd by our assumption, and at least one of $2^{-t}\alpha$ and $2^{-t}\alpha'$ is odd. If $2^{-t}\alpha'$ is odd, then both $2^{-t}\alpha$ and $\sum \ell'_j \zeta_j$ are odd, so $r = s$, and (†) is satisfied. Otherwise, $2^{-t}\alpha'$ is even, so $s > r$, $2^{-t}\alpha$ is odd and $\sum \ell'_j \zeta_j$ is even; thus (†) is satisfied. Therefore, by Kronecker's Theorem, the system of inequalities

$$|\theta_j \tau - (\delta + \zeta_j \pi)| < \epsilon \pmod{2\pi}, \qquad (\theta_j \in \Theta_{\mathbf{v}}).$$

admits a solution τ_0 for τ. Hence we obtain

$$U(\tau_0) = \sum_{\theta_j \in \Theta_{\mathbf{v}}} e^{i\tau_0 \theta_j} E_j = \sum_{\theta_j \in \Theta_{\mathbf{v}}} (1 - \epsilon') e^{i\delta} \sigma_j E_j$$

and so $U(\tau_0)\mathbf{v} \approx e^{i\delta}\mathbf{v}^\sigma$, and hence we have pretty good state transfer between states $\mathbf{v}$ and $\mathbf{v}^\sigma$.

Conversely, suppose that pretty good state transfer occurs between $\mathbf{v}$ and $\mathbf{v}^\sigma$. Applying Lemma 5.1.6, we see that for some τ, we have

$$\begin{aligned} U(\tau)\mathbf{v} &\approx e^{i\delta}\mathbf{v}^\sigma, \\ e^{i\theta_j \tau} E_j \mathbf{v} &\approx e^{i\delta} E_j \mathbf{v}^\sigma, && (\theta_j \in \Theta_{\mathbf{v}}), \\ e^{i\theta_j \tau} E_j \mathbf{v} &\approx (-1)^{j+1} e^{i\delta} E_j \mathbf{v}, && (\theta_j \in \Theta_{\mathbf{v}}), \\ \theta_j \tau &\approx \delta + \zeta_j \pi \pmod{2\pi}, && (\theta_j \in \Theta_{\mathbf{v}}). \end{aligned}$$

So by Kronecker's Theorem, for every set of integers $\{\ell_j\}$ such that $\sum \ell_j \theta_j = 0$, we have

$$\sum_{\theta_j \in \Theta_{\mathbf{v}}} \ell_j (\delta + \zeta_j \pi) \equiv 0 \pmod{2\pi}.$$

It follows that if $\sum \ell_j \zeta_j$ is odd, then $\sum \ell_j$ cannot be zero, or the above condition is not satisfied, which completes the proof. □

Next, we provide our key lemma, which uses cyclotomic polynomials to draw conclusions about the possible linear combinations of eigenvalues that equal zero, which will aid us in applying Kronecker's Theorem.

5.1.8 Lemma. *Let m be a positive integer of the form $2^t p^s$, where p is an odd prime and $s \in \mathbb{N}$, and let $\theta_j = 2\cos(j\pi/m)$, $1 \le j < m$. If there is a linear combination satisfying*

$$\sum_{j=1}^{m-1} \ell_j \theta_j = 0,$$

where each ℓ_j is an integer, then if $1 \le j \le m - m/p$, and we let $j := q(m/p) + r$, $0 \le r < m/p$, we have

$$\ell_j = \begin{cases} \ell_{m-j} + (-1)^q(\ell_{m-m/p+r} - \ell_{m/p-r}), & r \ne 0; \\ \ell_{m-j}, & r = 0. \end{cases}$$

Proof. Notice that each θ_j is of the form

$$\theta_j = \zeta_{2m}^{j} + \zeta_{2m}^{-j},$$

where ζ_{2m} is a $2m$-th primitive root of unity. Hence, every θ_j belongs to the cyclotomic field $\mathbb{Q}(\zeta_{2m})$. The cyclotomic polynomial is

$$\Phi_{2m}(x) = \sum_{k=0}^{p-1} (-1)^k x^{km/p}$$

and we define the polynomial $P(x)$ as follows:

$$P(x) = \sum_{j=1}^{m-1} \ell_j x^j + \sum_{m+1}^{2m-1} \ell_{2m-j} x^j.$$

We see that ζ_{2m} is a root of $P(x)$ and, since $\Phi_{2m}(x)$ is the minimal polynomial of ζ_{2m}, we see that $\Phi_{2m}(x)$ divides $P(x)$.

Let $Q(x)$ be the following polynomial:

$$Q(x) = \sum_{j=1}^{m/p} \ell_j x^j + \sum_{j=m/p+1}^{m-1} (\ell_j + \ell_{j-m/p})x^j + \ell_{m-m/p}x^m + \sum_{j=1}^{m/p-1} \left(\ell_{m-j} + \ell_{m-m/p+j} - \ell_j\right) x^{m+j}.$$

Now, as the degree of $Q(x)$ is $m + m/p - 1$, and

$$[x^j]\Phi_{2m}(x)Q(x) = [x^j]P(x), \quad 0 \le j \le m + m/p - 1,$$

we may conclude that $Q(x)$ is the unique polynomial of degree $m + m/p - 1$ such that $[x^j]\Phi_{2m}(x)Q(x) = [x^j]P(x)$ for $0 \le j \le m + m/p - 1$. In particular, the quotient $P(x)/\Phi_{2m}(x)$ is a polynomial of degree $m + m/p - 1$ with this property, and therefore $P(x) = \Phi_{2m}(x)Q(x)$. Hence, from the coefficients of x^{2m-j} for $1 \le j \le m - m/p$, we have

$$\ell_j = \begin{cases} \ell_{m-j} + (-1)^q(\ell_{m-m/p+r} - \ell_{m/p-r}), & r \neq 0; \\ \ell_{m-j}, & r = 0. \end{cases}$$

as desired. □

We also show that for states of paths of particular forms, we can draw conclusions about their eigenvalue supports. Recall we write $\mathbf{v} = \sum_{x \in V(P_n)} \beta_x \mathbf{e}_x$. If $\mathbf{v}$ is such that $\beta_x = 0$ for all even x, we say that $\mathbf{v}$ is an *odd state*, and if $\mathbf{v}$ is such that $\beta_x = 0$ for all odd x, we say that $\mathbf{v}$ is an *even state*. Moreover, we say a state is a *parity state* if it is an odd state or an even state.

5.1.9 Lemma. *For P_n, let $\mathbf{v}$ be a parity state. If $\theta_j \notin \Theta_{\mathbf{v}}$, then $\theta_{n+1-j} \notin \Theta_{\mathbf{v}}$.*

Proof. Let $\theta \in \Theta_{\mathbf{v}}$. Then for each $x \in V(P_n)$, we have

$$(E_j\mathbf{v})_x = \frac{2}{n+1}\left(\sin\frac{xj\pi}{n+1}\right)\sum_{y\in V(P_n)}\beta_y\left(\sin\frac{yj\pi}{n+1}\right) = 0.$$

Thus

$$\begin{aligned}(E_{n+1-j}\mathbf{v})_x &= \frac{2}{n+1}\left(\sin\frac{x(n+1-j)\pi}{n+1}\right)\sum_{y\in V(P_n)}\beta_y\left(\sin\frac{y(n+1-j)\pi}{n+1}\right)\\ &= \frac{2}{n+1}\left(-\cos(x\pi)\sin\frac{xj\pi}{n+1}\right)\sum_{y\in V(P_n)}\beta_y\left(-\cos(y\pi)\sin\frac{yj\pi}{n+1}\right)\\ &= \pm\frac{2}{n+1}\left(\sin\frac{xj\pi}{n+1}\right)\sum_{y\in V(P_n)}\beta_y\left(\sin\frac{yj\pi}{n+1}\right) = 0.\end{aligned}$$

Hence, $\theta_{n+1-j} \notin \Theta_{\mathbf{v}}$ as desired. □

We are now able to derive the following results, relating pretty good state transfer of states of paths to the eigenvalue support of the state.

5.1.10 Theorem. *Suppose $m = 2^t p^s$, where p is an odd prime and $s, t \in \mathbb{N}$, and let $\mathbf{v}$ be a parity state of P_{m-1}. For $1 \leq c < m/p$, let*

$$S_c := \{\theta_{c+jm/p} : 0 \leq j < p\}.$$

Moreover, let $S_0 := \{\theta_{m/2}\}$ be given. Then in P_{m-1}, there is pretty good state transfer between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if and only if there does not exist S_c with c odd and $S_{c'}$ with c' even such that $S_c \cup S_{c'} \subseteq \Theta_{\mathbf{v}}$.

Proof. First, suppose there exist S_c with c odd and $S_{c'}$ with c' even such that $S_c \cup S_{c'} \subseteq \Theta_{\mathbf{v}}$. Consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k = m/2 \text{ and } c = 0; \\ -1 & \text{if } k = m/2 \text{ and } c' = 0; \\ 1, & \text{if } k \equiv c \pmod{2m/p}, c \neq 0; \\ -1, & \text{if } k \equiv c + m/p \pmod{2m/p}, c \neq 0; \\ 1, & \text{if } k \equiv c' + m/p \pmod{2m/p}, c' \neq 0; \\ -1, & \text{if } k \equiv c' \pmod{2m/p}, c' \neq 0; \\ 0. & \text{otherwise.} \end{cases}$$

For $S_{m/2,m}$, we have that $\theta_{m/2} = 0$. Otherwise, by Lemma 4.3.2, we have that

$$\sum_{j=0}^{p-1} (-1)^j \theta_{c+jm/p} = \sum_{j=0}^{p-1} (-1)^j \cos\left(\frac{(c + jm/p)\pi}{m}\right) = 0,$$

and so $\sum_k \ell_k \theta_k = 0$. Moreover, we can verify that $\sum_k \ell_k \zeta_k$ is odd and $\sum_k \ell_k = 0$. Hence, by Theorem 5.1.7, we cannot have pretty good state transfer from $\mathbf{v}$.

Now, suppose we do not have S_c with c odd and $S_{c'}$ with c' even such that $S_c \cup S_{c'} \subseteq \Theta_{\mathbf{v}}$. Then $S_c \not\subseteq \Theta_{\mathbf{v}}$ for all odd c or $S_c \not\subseteq \Theta_{\mathbf{v}}$ for all even c. Consider $S_c \not\subseteq \Theta_{\mathbf{v}}$, $c \neq 0$. Then there exists a j_c such that $\theta_{c+j_c m/p} \notin \Theta_{\mathbf{v}}$, and by Lemma 5.1.9, we have that $\theta_{m-c-j_c m/p} \notin \Theta_{\mathbf{v}}$. So, in any linear combination, we assume $\ell_{c+j_c m/p} = \ell_{m-c-j_c m/p} = 0$. Therefore, letting $r_c \equiv c \pmod{m/p}$, $0 \leq r < m/p$, we have by Lemma 5.1.8 that $\ell_{m/p-r_c} = \ell_{m-m/p+r_c}$, and hence $\ell_j = \ell_{m-j}$ for every $j \equiv c \pmod{m/p}$.

Now, we first suppose $S_c \nsubseteq \Theta_{\mathbf{v}}$ for all odd c. Then it follows that $\ell_j = \ell_{m-j}$ for all odd j. Now suppose there is a set of integers $\{\ell_j\}$ such that $\sum_j \ell_j \theta_j = 0$ and $\sum_j \ell_j \zeta_j$ is odd. Then since the sum of the ℓ_j's for j odd is even, it follows that $\sum_j \ell_j \neq 0$. Hence, by Theorem 5.1.7, there is pretty good state transfer between $\mathbf{v}$ and $\mathbf{v}^\sigma$.

Next, we suppose $S_c \nsubseteq \Theta_{\mathbf{v}}$ for all even c. Then it follows, together with Lemma 5.1.8, that $\ell_j = \ell_{m-j}$ for all even j and $\ell_{m/2} = 0$. Hence, $\sum_j \ell_j \zeta_j$ is never odd. Hence, by Theorem 5.1.7, there is pretty good state transfer between $\mathbf{v}$ and $\mathbf{v}^\sigma$. □

5.1.11 Theorem. *Suppose $m = p^s$, where p is an odd prime and $s \in \mathbb{N}$, and let $\mathbf{v}$ be a parity state of P_{m-1}. For $1 \leq c < m/(2p)$, let*

$$R_c := \{\theta_{c+jm/p} : 0 \leq j < p\} \cup \{\theta_{m/p-c+jm/p} : 0 \leq j < p\}.$$

Then in P_{m-1}, there is pretty good state transfer between states $\mathbf{v}$ and $\mathbf{v}^\sigma$ if and only if there does not exist R_c such that $R_c \subseteq \Theta_{\mathbf{v}}$.

Proof. First, suppose there exists R_c such that $R_c \subseteq \Theta_{\mathbf{v}}$. Consider the set of integers $\{\ell_k\}$ given by

$$\ell_k = \begin{cases} 1, & \text{if } k \equiv c \pmod{2m/p} \text{ or } k \equiv 2m/p - c \pmod{2m/p}; \\ -1, & \text{if } k \equiv c + m/p \pmod{2m/p} \text{ or } k \equiv m/p - c \pmod{2m/p}; \\ 0, & \text{otherwise.} \end{cases}$$

By Lemma 4.3.2, we have that

$$\sum_{j=0}^{m/p-1} (-1)^j \theta_{c+jm/p} = \sum_{j=0}^{m/p-1} \cos\left(\frac{(c+jm/p)\pi}{m}\right) = 0,$$
$$\sum_{j=0}^{m/d-1} (-1)^j \theta_{m/p-c+jm/p} = \sum_{j=0}^{m/p-1} \cos\left(\frac{(m/p-c+jm/p)\pi}{m}\right) = 0,$$

and so $\sum_k \ell_k \theta_k = 0$. Moreover, we can verify that $\sum_k \ell_k \zeta_k$ is odd and $\sum_k \ell_k = 0$. Hence, by Theorem 5.1.7, we cannot have pretty good state transfer between $\mathbf{v}$ and $\mathbf{v}^\sigma$.

Now suppose there does not exist R_c such that $R_c \subseteq \Theta_{\mathbf{v}}$. Then for each c, there exists a c' such that $\theta_{c'} \in R_c \setminus \Theta_{\mathbf{v}}$, and by Lemma 5.1.9, we have that $\theta_{m-c'} \in R_c \setminus \Theta_{\mathbf{v}}$. So, in any linear combination, we assume $\ell_{c'} = \ell_{m-c'} = 0$. By Lemma 5.1.8, we have that $\ell_j = \ell_{m-j}$ for every $\theta_k \in R_c$. It follows, together with Lemma 5.1.8, that $\ell_j = \ell_{m-j}$ for every j. Now suppose there is a set of integers $\{\ell_j\}$ such that $\sum_j \ell_j \theta_j = 0$ and $\sum_j \ell_j \zeta_j$ is odd. Then it follows $\sum_j \ell_j \equiv 2 \pmod 4$, and in particular, is not zero. Hence, by Theorem 5.1.7, there is pretty good state transfer between $\mathbf{v}$ and $\mathbf{v}^\sigma$. □

As a consequence, we demonstrate pretty good state transfer in the following class.

5.1.12 Corollary. *Given any odd prime p and positive integer $t \geq 2$, there is pretty good state transfer in $P_{2^t p-1}$ between states $\mathbf{v} = \frac{1}{\sqrt{2}}(\mathbf{e}_a + \alpha \mathbf{e}_b)$ and $\mathbf{v}^\sigma = \frac{1}{\sqrt{2}}(\mathbf{e}_{2^t p-a} + \alpha \mathbf{e}_{2^t p-b})$ whenever $a \neq b$, $\alpha = \pm 1$, and $a + \alpha b \equiv 0 \pmod{2^t}$.*

Proof. We consider the eigenvalue support of $\mathbf{v}$. In particular, we show that $\theta_{2pj} \notin \Theta_{\mathbf{v}}$ for $1 \leq j < 2^{t-1}$. We have

$$\begin{aligned}
(E_{2pj}\mathbf{v})_x &= \frac{1}{\sqrt{2}}\left((E_{2pj})_{x,a} + \alpha (E_{2pj})_{x,b}\right) \\
&= \frac{2}{2^t p\sqrt{2}} \sin\left(\frac{jx\pi}{2^{t-1}}\right)\left(\sin\left(\frac{ja\pi}{2^{t-1}}\right) + \alpha \sin\left(\frac{jb\pi}{2^{t-1}}\right)\right) \\
&= \frac{4}{2^t p\sqrt{2}} \sin\left(\frac{jx\pi}{2^{t-1}}\right) \sin\left(\frac{j(a+\alpha b)\pi}{2^t}\right) \cos\left(\frac{j(a-\alpha b)\pi}{2^t}\right) = 0,
\end{aligned}$$

since $a+\alpha b$ is a multiple of 2^t. We observe that $2p$ generates the subgroup $\{0, 2, 4, \ldots, 2^t-2\}$ of $\mathbb{Z}_{2^t}$. Moreover, we have shown that $\theta_{2^{t-1}p} \notin \Theta_{\mathbf{v}}$. Hence, for every even c, we have that $S_c \not\subseteq \Theta_{\mathbf{v}}$, and so by Theorem 5.1.10, there is pretty good state transfer between $\mathbf{v}$ and $\mathbf{v}^\sigma$. □

5.2 Fractional Revival

Fractional revival can be viewed as another special case of state transfer on graphs, where we start with a single vertex state and desire transfer to a subset of the vertices of the graph, including the initial vertex. Formally, we say a graph X has *fractional revival* from vertices a to b at time $\tau \in \mathbb{R}$ if for some $\alpha, \beta \in \mathbb{C}$ with $|\alpha|^2 + |\beta|^2 = 1$ and $\beta \neq 0$, we have

$$U(\tau)\mathbf{e}_a = \alpha \mathbf{e}_a + \beta \mathbf{e}_b.$$

We additionally say that X has (α, β)-revival from a to b at time τ. Notice that if we have $\beta = 0$, then such a definition would mean a is periodic, and this case is excluded from the definition, as otherwise periodicity at a would imply fractional revival between a and every other vertex. On the other hand, if $\alpha = 0$, then such a definition would mean there is perfect state transfer between a and b, and this is allowed to be an example of fractional revival. Moreover, for a graph X, a vertex a, and a subset of the vertices $B \ni a$, we say X has *generalized fractional revival* from a to B at time $\tau \in \mathbb{R}$ if $\mathbf{e}_b^T U(\tau)\mathbf{e}_a \neq 0$ if and only if $b \in B$.

Fractional revival in weighted graphs was introduced by Chen, Song, and Sun [11] and further studied by Banchi, Compagno, and Bose [3], Genest, Vinet, and Zhedanov [27], and Christandl, Vinet, and Zhedanov [19]. It was considered for the unweighted graph by Chan et al. [10]. In what follows, we provide a survey of their main results. We begin by stating a few constructions of fractional revival from perfect state transfer, periodicity, and uniform mixing.

5.2.1 Theorem. *[10] Let X be a graph that is periodic at vertex a at time τ. Let Y be a graph with instantaneous uniform mixing at time τ. Then, for any vertex u of Y, the graph $X \square Y$ has generalized fractional revival from (a, u) to the vertices $\{(a, v) : v \in V(Y)\}$ at time τ.*

5.2.2 Theorem. *[10] Let X be a graph with perfect state transfer between vertices a and b at time τ, where $\tau < \pi/2$. Let Y be a graph on the same vertex set as X where (a, b) is an isolated edge. If the adjacency matrices of X and Y commute, then $X \cup Y$ has fractional revival at time τ.*

5.2.3 Theorem. *[10] Suppose Y has perfect state transfer between vertices a and b at time $\pi/2$. Assume there is an automorphism T of Y with order two which swaps a and b. Consider the graph X_θ whose adjacency matrix is*

$$A(X_0) = I \otimes A(Y) + \cos(2\theta)(\sigma_X \otimes I) + \sin(2\theta)(\sigma_Z \otimes T).$$

(Note: $X_0 = K_2 \square Y$.) Then X_θ has $e^{-i\pi/2}(\sin(2\theta), \cos(2\theta))$-revival between $(0, a)$ and $(1, b)$ at time $\pi/2$.

We now present their result demonstrating a sort of symmetry property for fractional revival from a to b and b to a, albeit with different parameters.

5.2.4 Proposition. *[10] If (α, β)-revival occurs from a to b in a graph X then $(-\frac{\overline{\alpha}\beta}{\overline{\beta}}, \beta)$-revival occurs from b to a at the same time.*

Similarly to state transfer, they demonstrate that the vertices involved in fractional revival must be parallel.

5.2.5 Proposition. *[10] If there is (α, β)-revival between a and b in a graph X, then these vertices are parallel.*

On the other hand, the vertices involved need not be cospectral. However, if the vertices involved are also cospectral, more can be said about the eigenvalues of the graph, similarly to the characterization of periodicity at a vertex (Theorem 3.2.7).

5.2.6 Theorem. *[10] Assume X admits fractional revival between strongly cospectral vertices a and b. Let $\theta_0, \ldots, \theta_t$ be the eigenvalues in their support. Then these are either integers or quadratic integers. Moreover, there are integers a^+, a^-, Δ^+ (square-free), Δ^- (square-free), and $\{b_r\}_{r=0}^t$ such that, for all $r = 0, \ldots, t$,*

(a) if $\sigma_r = 1$, then $\theta_r = \frac{a^+ + b_r\sqrt{\Delta^+}}{2}$, and

(b) if $\sigma_r = -1$, then $\theta_r = \frac{a^- + b_r\sqrt{\Delta^-}}{2}$.

Moreover, when the vertices being considered are strongly cospectral, fractional revival occurs together with perfect state transfer, pretty good state transfer, or periodicity.

5.2.7 Theorem. *[10] If fractional revival occurs between two strongly cospectral vertices a and b in X, then X has perfect state transfer or pretty good state transfer from a to b, or X is periodic at a and b at the same time.*

The next result compares fractional revival in a graph with fractional revival in its quotient. We define an *equitable partition* $\rho = \bigcup_i C_i$ to be a partition of the vertex set of a graph X such that for every i, j, all vertices in C_i have the same number of neighbours d_{ij} in C_j. Then the *quotient graph* X/ρ has vertex set ρ and the edge joining C_i and C_j has weight $\sqrt{d_{ij}d_{ji}}$.

5.2.8 Theorem. *[10] Suppose a graph X has an equitable partition ρ containing singleton cells $\{a\}$ and $\{b\}$. There is fractional revival between a and b in X if and only if there is fractional revival between $\{a\}$ and $\{b\}$ in the quotient X/ρ.*

Next, while strong cospectrality is not a requirement for fractional revivial, a stronger condition than parallel is needed, as the following proposition shows. We let $\mathsf{Aut}_X(a)$ denote the group of automorphisms that fix the vertex a.

5.2.9 Proposition. *[10] Suppose fractional revival occurs between a and b in a graph X, then $\mathsf{Aut}_X(a) = \mathsf{Aut}_X(b)$.*

For a bipartite graph, stronger conditions are also obtained which depend on whether the two vertices are in the same colour class.

5.2.10 Theorem. *[10] Suppose (α, β)-revival occurs between a and b in a bipartite graph X at time τ. If a and b belong to different colour classes of X then a and b are strongly cospectral. If a and b belong to the same colour class then X is periodic at both vertices at time 2τ.*

Finally, fractional revival is characterized for cycles and paths.

5.2.11 Theorem. *[10] Fractional revival occurs in a cycle if and only if it has four or six vertices.*

5.2.12 Theorem. *[10] A path P_n admits fractional revival if and only if $n \in \{2, 3, 4\}$.*

5.3 Future Directions

We would like to continue the characterization of pretty good state transfer of multiple qubit states in terms of the eigenvalue support for cases when the length of the path is not of the form $2^t p^s - 1$ or when the initial state is not a parity state. One of the challenges with considering other lengths is that the cyclotomic polynomial does not have as elegant a form as those we considered, and so it seems less likely that removing a small number of eigenvalues would lead to the same symmetry of coefficients that we obtain in these cases. For example, the 30th cyclotomic polynomial is

$$x^8 + x^7 - x^5 - x^4 - x^3 + x + 1,$$

and later polynomials will have coefficients other than 1, 0, and -1. For initial states which are not parity states, we lose the property that θ is in the eigenvalue support of the state if and only if $-\theta$ is, so we would again need to expand our consideration of what eigenvalue supports would allow pretty good state transfer.

Additionally, Vieira and Rigolin [46] analyzed numerically the transfer of entanglement when the path is modified by adding an additional leaf at each end and changing the edge weights, and considering transfer between the pairs of leaves. We are interested in pursuing this problem analytically, and to determine if the length of the path has a similar influence as the single state case. We would also like to compare the performance of pretty good state transfer in this case, to pretty good state transfer of the first two vertices of the path, and motivated by our results for parity states, the first and third vertices of a path, to determine whether modify the path provides any advantage.

Finally, the results for pretty good state transfer of parity states on paths and the results for fractional revival are both examples of multiple qubit state transfer. We would like to investigate whether there is a more general class of examples of pretty good state transfer, particularly for paths, that captures both of these ideas. Such a generalization may also allow us to expand our results for either of these problems.

References

[1] D. Aharonov, A. Ambainis, J. Kempe, and U. Vazirani, *Quantum walks on graphs*, Proceedings of the Thirty-Third Annual ACM Symposium on Theory of Computing - STOC '01 (2001), 50–59.

[2] A. Ahmadi, R. Belk, C. Tamon, and C. Wendler, *On mixing in continuous-time quantum walks on some circulant graphs*, Quantum Information & Computation **3** (2003), no. 6, 611–618.

[3] L. Banchi, E. Compagno, and S. Bose, *Perfect wave-packet splitting and reconstruction in a one-dimensional lattice*, Physical Review A **91** (2015), no. 5, 052323.

[4] L. Banchi, G. Coutinho, C. Godsil, and S. Severini, *Pretty good state transfer in qubit chains — the Heisenberg Hamiltonian*, Journal of Mathematical Physics **58** (2017), no. 3, 032202.

[5] N. Biggs, *Algebraic Graph Theory*, Cambridge University Press, Cambridge, 1974.

[6] S. Bose, *Quantum communication through an unmodulated spin chain*, Physical Review Letters **91** (2003), no. 20, 207901.

[7] D. Bump, *Lie Groups*, Springer, New York, 2013.

[8] D. Burgarth, *Quantum State Transfer with Spin Chains*, Ph.D. Thesis, University College London, 2007.

[9] S. Cameron, S. Fehrenbach, L. Granger, O. Hennigh, S. Shrestha, and C. Tamon, *Universal state transfer on graphs*, Linear Algebra and its Applications **455** (2014), 115–142.

[10] A. Chan, G. Coutinho, C. Tamon, L. Vinet, and H. Zhan, *Quantum fractional revival on graphs*, Discrete Applied Mathematics (2019), https://doi.org/10.1016/j.dam.2018.12.017.

[11] B. Chen, Z. Song, and C.P. Sun, *Fractional revivals of the quantum state in a tight-binding chain*, Physical Review A **75** (2007), no. 1, 012113.

[12] A. M. Childs, *Universal computation by quantum walk*, Physical Review Letters, **102** (2009), no. 18, 180501.

[13] A. M. Childs, R. Cleve, E. Deotto, E. Farhi, S. Gutmann, and D. A. Spielman, *Exponential algorithmic speedup by quantum walk*, Proceedings of the Thirty-Third Annual ACM Symposium on Theory of Computing (2003), 59–68.

[14] A. M. Childs, E. Farhi, and S. Gutmann, *An example of the difference between quantum and classical random walks*, Quantum Information Processing **1** (2002), no. 1-2, 35–43.

[15] A. M. Childs and J. Goldstone, *Spatial search and the Dirac equation*, Physical Review A **70** (2004), no. 4, 042312.

[16] A. M. Childs and J. Goldstone, *Spatial search by quantum walk*, Physical Review A **70** (2004), no. 2, 022314.

[17] M. Christandl, N. Datta, T. C. Dorlas, A. Ekert, A. Kay, and A. J. Landahl, *Perfect transfer of arbitrary states in quantum spin networks*, Physical Review A **71** (2005), no. 3, 032312.

[18] M. Christandl, N. Datta, A. Ekert, and A. J. Landahl, *Perfect state transfer in quantum spin networks*, Physical Review Letters **92** (2004), no. 18, 187902.

[19] M. Christandl, L. Vinet, and A. Zhedanov, *Analytic next-to-nearest-neighbor XX models with perfect state transfer and fractional revival*, Physical Review A **96** (2017), no. 3, 032335.

[20] G. Coutinho and C. Godsil, *Graph Spectra and Continuous Quantum Walks*, Unpublished, 2019.

[21] G. Coutinho, K. Guo, and C. M. van Bommel, *Pretty good state transfer between internal nodes of paths*, Quantum Information & Computation **17** (2017), no. 9-10, 825–830.

[22] G. Coutinho and H. Liu, *No Laplacian perfect state transfer in trees*, SIAM Journal on Discrete Mathematics **29** (2015), no. 4, 2179–2188.

[23] G. Coutinho, *Quantum State Transfer in Graphs*, Ph.D. Thesis, University of Waterloo, 2014.

[24] X. Fan and C. Godsil, *Pretty good state transfer on double stars*, Linear Algebra and its Applications **438** (2013), no. 5, 2346–2358.

[25] E. Farhi and S. Gutmann, *Analog analogue of a digital quantum computation*, Physical Review A **57** (1998), no. 4, 2403.

[26] E. Farhi and S. Gutmann, *Quantum computation and decision trees*, Physical Review A **58** (1998), no. 2, 915.

[27] V. Genest, L. Vinet, and A. Zhedanov, *Quantum spin chains with fractional revival*, Annals of Physics **371** (2016), 348–367.

[28] H. Gerhardt and J. Watrous, *Continuous-time quantum walks on the symmetric group*, Proceedings of the 7th International Workshop on Randomization and Approximation Techniques in Computer Science, (2003).

[29] C. Godsil, *Algebraic Combinatorics*, Chapman & Hall, New York, 1993.

[30] C. Godsil, *Periodic graphs*, The Electronic Journal of Combinatorics **18** (2011), no. 1, 23.

[31] C. Godsil, *Controllable subsets in graphs*, Annals of Combinatorics **16** (2012), no. 4, 733–744.

[32] C. Godsil, *State transfer on graphs*, Discrete Mathematics **312** (2012), no. 1, 129–147.

[33] C. Godsil, *When can perfect state transfer occur?* Electronic Journal of Linear Algebra **23** (2012), no. 1, 62.

[34] C. Godsil, S. Kirkland, S. Severini, and J. Smith, *Number-theoretic nature of communication in quantum spin systems*, Physical Review Letters **109** (2012), no. 5, 050502.

[35] C. Godsil and G. F. Royle, *Algebraic Graph Theory*, Springer New York, 2001.

[36] C. Godsil and J. Smith, *Strongly cospectral vertices*, arXiv:1709.07975 (2017).

[37] A. Kay, *The basics of perfect communication through quantum networks*, arXiv:1102.2338 (2011).

[38] B. M. Levitan and V. V. Zhikov, *Almost Periodic Functions and Differential Equations*, Cambridge University Press, 1982.

[39] C. Moore and A. Russell, *Quantum walks on the hypercube*, In International Workshop on Randomization and Approximation Techniques in Computer Science, Springer, Berlin, Heidelberg, 2002.

[40] M. A. Neilsen and I. L. Chuang, *Quantum Computation and Quantum Information*, Cambridge University Press, Cambridge, 2010.

[41] N. Saxena, S. Severini, and I. E. Shparlinski, *Parameters of integral circulant graphs and periodic quantum dynamics*, International Journal of Quantum Information **5** (2007), no. 03, 417–430.

[42] A. J. Schwenk, *Almost all trees are cospectral*, New Directions in the Theory of Graphs (1973), 275–307.

[43] R. Sousa and Y. Omar, *Pretty good state transfer of entangled states through quantum spin chains*, New Journal of Physics **16** (2014), no. 12, 123003.

[44] D. Stevanovic, *Applications of graph spectra in quantum physics*, Selected Topics in Applications of Graph Spectra (2011), 85–111.

[45] C. M. van Bommel, *A complete characterization of pretty good state transfer on paths*, Quantum Information & Computation **19** (2019), no. 7-8, 601–608.

[46] R. Vieira and G. Rigolin, *Almost perfect transport of an entangled two-qubit state through a spin chain*, Physics Letters A **382** (2018), no. 36, 2586–2594.

[47] L. Vinet and A. Zhedanov, *Almost perfect state transfer in quantum spin chains*, Physical Review A **86** (2012), no. 5, 052319.

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