Edge State Transfer

by

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A thesis
presented to the University of Waterloo
in fulfillment of the
thesis requirement for the degree of
Master of Mathematics
in
Combinatorics and Optimization

Waterloo, Ontario, Canada, 2018

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

Let G be a graph and let t be a positive real number. Then the evolution of the continuous quantum walk defined on G is described by the transition matrix

$$U(t) = \exp(itH).$$

The matrix H is called Hamiltonian. So far the most studied quantum walks are the ones whose Hamiltonians are the adjacency matrices of the underlying graphs and initial states are vertex states e_a, with e_a being the characteristic vector of vertex a.

This thesis focuses on Laplacian edge state transfer, that is, the quantum walks whose initial states are edge states $e_a - e_b$ and Hamiltonians are the Laplacians of the underlying graphs. So far the research about perfect state transfer only involves vertex states and Laplacian edge state transfer has not been studied before. We extend the known results of perfect vertex state transfer and periodicity of vertex states to Laplacian edge state transfer.

We prove two useful closure properties for perfect Laplacian edge state transfer. One is that complementation preserves perfect edge state transfer. The other is that if G has perfect Laplacian edge state transfer at time τ and H has perfect Laplacian vertex state transfer also at time τ, then with some mild assumption on the pairs of vertex states and edge states that have perfect state transfer, the Cartesian product $G \square H$ also admits perfect edge state transfer. Those two properties provide us new ways to construct graphs with perfect Laplacian edge state transfer. We also observe one phenomenon that happens in Laplacian edge state transfer which never happens in vertex state transfer: if there is perfect state transfer from $e_a - e_b$ to $e_\alpha - e_\beta$ and also from $e_b - e_c$ to $e_\beta - e_\gamma$ at the same time t in G, then G admits perfect state transfer from $e_a - e_c$ to $e_\alpha - e_\gamma$ at time t.

We give characterizations of perfect Laplacian edge state transfer in cycles, paths and complete bipartite graphs $K_{2,4n}$. We study perfect state transfer and periodicity on edge states with special spectral features. We also consider the case when the unsigned Laplacian is Hamiltonian and initial states are plus states of the form $e_a + e_b$. In this case, we characterize perfect state transfer in paths, cycles and bipartite graphs. We close this thesis by a list of open questions.

Acknowledgements

I would like to thank my supervisor, Chris Godsil, for his guidance and encouragement through my master's studies. Thank you for always being patient, supportive and optimistic.

I would like to thank David Gosset and David Wagner for reading my thesis and for their helpful feedbacks.

Also, thank my friends in the C&O department for keeping my company.

Lastly, I would like to thank my parents for their unconditional love and support.

Contents

Chapter 1

Introduction

Continuous time quantum walks were first introduced by Farhi and Gutmann [10] in 1998. Exploiting the interference effects of quantum mechanics, quantum walks outperform classical random walks for some computational tasks. In 2002, for a certain black-box problem, Childs et al. [4] proposed a graph where continuous quantum walks promise an exponential speedup over any classical computations.

The concept of quantum state transfer was proposed by Bose [2] in 2003. Later in the field of quantum information processing, Christandl et al. [6] brought our attention to the topic of perfect state transfer. In 2008, using the tool of quantum scattering theory, Childs [3] proved that continuous time quantum walk can be regarded as a universal computational primitive and any desired quantum computation can be encoded in some underlying graph of the quantum walk. Quantum walks have become powerful tools to improve existing quantum algorithms and develop new quantum algorithms.

A quantum walk is a quantum mechanical analogue of a classical random walk. A qubit is a quantum analogue of a classical bit. We associate a qubit with a 2-dimensional vector space over $\mathbb{C}$. The state of a qubit is a 1-dimensional subspace from a 2-dimensional complex vector space. One way to represent states of qubits is using unit vectors and two states x, y are equivalent if

$$x = \gamma y$$

for some complex scalar γ of norm 1. Physicists call γ a phase factor. We can also represent states of qubits using the projections in the form of

$$\frac{1}{x^* x} x x^*$$

where x is a non-zero vector and x^* is the conjugate transpose of x. Two states x, y are equivalent if

$$\frac{1}{x^*x}xx^* = \frac{1}{y^*y}yy^*.$$

This is consistent with the unit vector representation of states when x, y are unit vectors and we can get rid of our phase factors.

Following the mathematical interpretation due to Coutinho and Godsil [8], the evolution of a quantum walk is described by its transition matrix

$$U(t) = \exp(itH),$$

where Hermitian matrix H is called a "Hamiltonian". Density matrices are positive semidefinite with trace 1 and we can use density matrices to represent states of our quantum system. Let P, Q denote two states of a quantum walk. There is perfect state transfer from P to Q at time t if

$$U(t)PU(t)^* = Q,$$

and a state is periodic if there is a time t such that it has perfect state transfer to itself at time t.

Let G be a graph with n vertices. The *adjacency matrix* $A(G)$ of G is a symmetric 01-matrix of order $n \times n$ whose rows and columns are indexed by vertices of G and

$$A(G)_{uv} = \begin{cases} 1 & \text{if } (u,v) \in E(G), \\ 0 & \text{otherwise.} \end{cases}$$

The *degree matrix* $\Delta(G)$ of G is a diagonal matrix of order $n \times n$ whose rows and columns are indexed by vertices of G and

$$\Delta(G)_{ii} = \deg(i).$$

For a quantum walk defined over G, so far the most studied case is adjacency vertex state transfer. That is the case when the Hamiltonian is the adjacency matrix A of G with initial state associated with a vertex of G. That is, the transition matrix is

$$U(t) = \exp(itA)$$

and the initial state is a vertex state e_v, where $e_v \in \mathbb{R}^n$ is the characteristic vector of vertex v. We also can use density matrix

$$P = e_v e_v^T$$

to represent a vertex state. However, perfect state transfer as a significant phenomenon in quantum communication is very rare in this setting. As stated above, the initial states of quantum walks can also be represented by density matrices, which gives a new approach to find perfect state transfer in graphs.

Finding more graphs where the overlying quantum walks can have perfect state transfer is the main motivation of this thesis. So far all the researches have been done about perfect state transfer involving only vertex states. We hope that using different forms of the initial state and different Hamiltonians can help us to get more perfect state transfer in graphs, which turns out to be effective.

In this thesis, we focus on the case when the initial state is an edge state. That is, the initial state is in the form

$$\frac{1}{\sqrt{2}}(e_a - e_b)$$

whose corresponding density matrix is

$$\frac{1}{2}(e_a - e_b)(e_a - e_b)^T.$$

Notice that the Laplacian of G is

$$\Delta(G) - A(G) = \sum_{(a,b)\in E(G)} \frac{1}{2}(e_a - e_b)(e_a - e_b)^T.$$

In this case, we use the Laplacian of G as Hamiltonian to describe the continuous quantum walks defined over G. Computations in `SAGE` tell us that perfect state transfer is still rare in Laplacian edge state transfer. But compared to vertex state transfer using adjacency matrices as Hamiltonians, there is a significant increase in terms of the number of periodic states over the same set of graphs. One can refer to Table 2.1 and Table 2.2 for details. As a special case of Laplacians, we also study quantum walks when the unsigned Laplacians $\Delta(G) + A(G)$ of underlying graphs are Hamiltonian. In this case, our initial state is called plus state with the form

$$\frac{1}{\sqrt{2}}\,(e_a + e_b)$$

with the corresponding density matrix

$$\frac{1}{2}(e_a + e_b)(e_a + e_b)^T.$$

The main tool used in this thesis is algebraic graph theory. Spectral decompositions of Hamiltonians provide us a strong connection between continuous quantum walks and spectral properties of the underlying graph. Through out this thesis, all the graphs are finite, simple and undirected.

The most investigated quantum walks on graphs are using the adjacency matrices as Hamiltonian and vertex states serve as initial states. Most of earlier works are proved using vertex state e_v as initial states. To the best of the author's knowledge, Laplacian edge state transfer has not been studied before, which lead to a sparse list of references we can rely on. We prove earlier results in vertex state transfer using density matrices in Chapter 3, which means that analogous results hold for edge states and plus states as well. This allows us to extend those basic but important results in vertex state transfer to Laplacian edge state transfer and unsigned Laplacian plus state transfer.

We prove the properties of symmetry and monogamy of perfect edge state transfer in Section 3.1. There is perfect state transfer from P to Q at time t if and only if there is perfect state transfer from Q to P at the same time t. Perfect state transfer from P happens at exactly half of the period of P, which implies that perfect state transfer is monogamous. Being periodic is necessary for an edge state to have perfect edge state transfer. The ratio condition holds for periodic edge state, which implies that the spectral properties of the graph can determine periodicity of a state (Section 3.2). Those are the most fundamental results we borrowed from vertex state transfer and we also adapt some useful algebraic results in the context of edge state transfer in Section 3.4.

To have more perfect state transfer, we study the constructions that can preserve perfect state transfer. We prove a closure property of Laplacian edge state transfer.

4.1.2 Theorem. *There is a perfect state transfer between* $e_a - e_b$ *and* $e_c - e_d$ *in graph* G *if and only if there is perfect state transfer between* $e_a - e_b$ *and* $e_c - e_d$ *in the complement* $\overline{G}$.

The Cartesian product of G and a graph H also can have perfect state transfer as long as H satisfies some certain condition (Theorem 4.2.3). Those two graph operations help us to construct new graphs admitting perfect edge state transfer. The author also observes the phenomenon of transitivity when perfect edge state transfer occurs under certain conditions.

4.3.1 Theorem. *Suppose there is perfect state transfer between* $e_a - e_b$ *and* $e_\alpha - e_\beta$ *at time* τ *in* G *and there is also perfect state transfer between* $e_b - e_c$ *and* $e_\beta - e_\gamma$ *at the same time* τ *in* G. *Then there is perfect state transfer between* $e_a - e_c$ *and* $e_\alpha - e_\gamma$ *at time* τ *in* G.

This transitivity phenomenon can never happen in vertex state transfer due to the restricted form of vertex states.

We also look into three classes of graphs, i.e., paths, cycles, bipartite graphs, that admit perfect edge/plus state transfer in Chapter 5 and Chapter 6. Due to the similarity of the Laplacian and the unsigned Laplacian of a bipartite graph, Laplacian edge state transfer and unsigned Laplacian plus state transfer on bipartite graphs are essentially the same.

For a regular graph, the transition matrices determined by the adjacency matrices, Laplacians and unsigned Laplacians are all equivalent, up to some phase factor. Our studies of state transfer on cycles also confirm this. It is easy to verify that C_4 has perfect vertex state transfer between its antipodal vertices. We get analogue results for Laplacian edge state transfer and unsigned Laplacian plus state transfer. The only cycle that has perfect edge state transfer is C_4 and it happens between the opposite edges. We proved similar conclusion for unsigned Laplacian plus state transfer as well. Here we can see that with equivalent transition matrices, different choices of initial state do not play a big role.

Stevanović [17] and Godsil [12] show that paths P_2, P_3 are the only paths that perfect vertex state transfer occurs and they occurs between the end-vertices of P_2, P_3. In this thesis, we also study Laplacian edge state transfer and unsigned Laplacian plus state transfer on paths.

5.4.7 Theorem. *A path graph on* n *vertices has perfect edge state transfer if and only if* $n = 3$ *or* 4.

6.2.7 Theorem. *A path graph on n vertices has perfect plus state transfer if and only if $n = 3$ or 4.*

Notice that the line graphs of P_3, P_4 are P_2, P_3 respectively. Perfect vertex state transfer on P_2 and perfect Laplacian edge state transfer as well as perfect unsigned Laplacian plus state transfer on P_3 all occurs at the same time $\pi/2$. Also, perfect state transfer on P_3 and perfect Laplacian edge state transfer as well as perfect unsigned Laplacian plus state transfer on P_4 all occurs at the same time $\pi/2$. But in general, there is no direct correspondence between vertex state transfer on a graph and edge/plus state transfer on its line graph.

Despite all the similarities that adjacency vertex state transfer, Laplacian edge state transfer and unsigned Laplacian plus state transfer share, Tables 2.1, 2.2, 6.1 show us that different choices of initial states and Hamiltonian can cause a huge gap in the number of periodic states, which largely affect the number of states that have perfect state transfer. The author has not been able to unfold the cause of the gaps. There are still a lot of open questions and we list them in the last chapter.

Chapter 2

Background

The purpose of this chapter is to provide sufficient background for the rest of this thesis. We start with introducing the physics background on continuous-time quantum walks from a mathematical perspective. Hamiltonians govern the dynamics of quantum systems and hence, we will spend a section to study two often used Hamiltonians in continuous quantum walks. Transition matrices describe quantum operations on quantum states. We will study some basic properties of transition matrices to help us get a better understanding of quantum walks.

Next, we introduce the algebraic tools we use in this thesis to study quantum state transfer and show how it can be applied to quantum walks. Following this, we introduce edge state transfer, which is the main concern of thesis. We explore some nice properties of eigenvalue support whose role in quantum walks is critical. Last, comparing vertex state transfer with edge state transfer, we will show some computational results and reveal possible advantages that edge state transfer can have, which hopefully can motivate readers to study edge state transfer.

We start by defining some basic concepts in quantum walks using mathematical language, which is provided by Coutinho and Godsil in [8].

A *quantum system* is a finite dimensional vector space over $\mathbb{C}$, with the inner product

$$\langle x, y\rangle := x^* y$$

in which x^* is the conjugate transpose of x. A *qubit* is a quantum system with dimension two, which is the basic unit in quantum information. The one-dimensional subspaces of a quantum system are the *states* of the system. If x and y are two unit vectors that span the same 1-dimensional subspace, then there is a complex scalar γ of norm 1 such that

$$y = \gamma x.$$

Physicists refer to γ as a *phase factor*.

Any physical process on a quantum system is necessarily determined by a unitary operator U and the measurement of a system is specified by a Hermitian operator H. We carry out the measurement to know which eigenspace of H the system is in. To perform a measurement on a quantum system with m-dimension, we must choose an orthogonal basis of H. It is conventional to use the standard basis $e_1, e_2, \cdots, e_m$ and the outcome of a measurement is an element of $\{1, 2, \cdots, m\}$.

If our system is in the state represented by a unit vector z, then when we measure the system with H, the outcome is r with probability

$$|\langle e_r, z \rangle|^2,$$

which is the r-th entry of the vector $z \circ \bar{z}$. If M, N are two matrices of order $n \times n$, then their Schur product $M \circ N$ is a matrix of order $n \times n$ such that

$$(M \circ N)_{i,j} = M_{i,j} N_{i,j}.$$

The schur product $z \circ \bar{z}$ contains all the information that a measurement can provide and the r-th entry z_r is determined up to a phase factor.

2.1 Quantum Walks

The concept of a quantum walk was introduced by Farhi and Gutmann [10] in 1998 as a quantum mechanical analogue of a classical random walk on decision trees. A classical algorithm is to run a random walk on a tree initialized at the root, to decide whether the tree contains a node at level n from the root. Farhi and Gutmann devised a quantum mechanical algorithm that evolves a state, initialized at a root through the tree, which can provide significant speed-up over the classical algorithm.

In 2004, to solve problems in quantum information processing, Christandl et al. [6] proposed the problem of finding perfect state transfer in quantum spin networks. A quantum spin network can be generally viewed as a collection of interacting qubits on a graph. Since then, there is a large amount of attention addressed to the subject of perfect state transfer and we will also pay close attention to this subject [5], [16], [11].

We use graphs to represent networks of interacting qubits and study quantum state transfer during quantum communication over the network. Let G be a graph. A *continuous-time quantum walk* or *continuous quantum walk* on G is described by its *transition matrix*, i.e.,

$$U(t) = \exp(itH),$$

where H denotes the suitable Hamiltonian associated to G. Note that physicists usually define the transition matrix as

$$U(t) = \exp(-itH).$$

We will show later on that we only care about the matrix

$$U(t) \circ U(-t)$$

in this thesis, so we use

$$U(t) = \exp(itH)$$

to be our definition of transition matrices for convenience.

2.2 Hamiltonians

We can see that the choice of Hamiltonian determines the dynamics of a quantum spin network. Here, we introduce two time-independent Hamiltonians in quantum walks, that is, XY-Hamiltonian and XYZ-Hamiltonian. The main sources for this section are Coutinho and Godsil [8, Section 2.5]. One can also refer to Christandl et al. [6] for more details in physics.

Let G be a graph on n vertices and each vertex of G is assigned to a qubit that is two-dimensional vector space over $\mathbb{C}$. Thus, the state space of a quantum walk on G is isomorphic to $(\mathbb{C}^2)^{\otimes n}$. Let e_0, e_1 denote the standard basis vectors of $\mathbb{C}^2$. If $S \subseteq V(G)$, we define

$$e_S = e_{i(1)} \otimes e_{i(2)} \otimes \cdots \otimes e_{i(n)},$$

where

$$\begin{cases} i(u) = 1 & \text{if } u \in S \\ i(u) = 0 & \text{if } u \notin S \end{cases}.$$

Let $\sigma^x, \sigma^y, \sigma^z$ be the Pauli matrices such that

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For a vertex $u \in V(G)$ and $w \in \{x, y, z\}$, we define an operator

$$\sigma_u^w = I_2 \otimes I_2 \otimes \cdots \otimes I_2 \otimes \sigma^w \otimes I_2 \otimes \cdots \otimes I_2,$$

where the u-th position is σ^w and the identity everywhere else. Note that

$$\sigma^x e_0 = e_1, \quad \sigma^x e_1 = e_0, \quad \sigma^y e_0 = ie_1, \quad \sigma^y e_1 = ie_0,$$

and

$$\sigma^z e_0 = e_0, \quad \sigma^z e_1 = -e_1.$$

Thus, if $a \neq b$ and $S \oplus T$ denote the symmetric difference of S and T, we have that

$$\sigma_a^x \sigma_b^x e_S = e_{S \oplus \{a,b\}}, \quad \sigma_a^y \sigma_b^y e_S = -(-1)^{|S \cap \{a,b\}|} e_{S \oplus \{a,b\}}$$

as well as

$$\sigma_a^z \sigma_b^z e_S = (-1)^{|S \cap \{a,b\}|} e_S.$$

There are two often used Hamiltonians in continuous quantum walks, that is, the XY-Hamiltonian and the XYZ-Hamiltonian. The *XY-Hamiltonian* is defined as

$$H_{XY} = \frac{1}{2} \sum_{\{a,b\} \in E(G)} \left(\sigma_a^x \sigma_b^x + \sigma_a^y \sigma_b^y \right)$$

and the *XYZ-Hamiltonian* is

$$H_{XYZ} = \frac{1}{2} \sum_{\{a,b\} \in E(G)} \left(\sigma_a^x \sigma_b^x + \sigma_a^y \sigma_b^y + \sigma_a^z \sigma_b^z \right).$$

To understand the image of e_S under H_{XY}, we introduce the k-th symmetric power $G^{\{k\}}$ of a graph G. The k-th symmetric graph $G^{\{k\}}$ has the k-subsets of $V(G)$ as vertices and two k-subsets are adjacent if their symmetric difference is an edge of G.

2.2.1 Theorem. *The matrix that represents the action of H_{XY} on the span of a vector e_S with $|S| = k$ is the adjacency matrix of the k-th symmetric power of the graph G.*

Proof. For an edge $a, b \in E(G)$, we have

$$\begin{aligned}\frac{1}{2}\left(\sigma_a^x\sigma_b^x + \sigma_a^y\sigma_b^y\right) e_S &= \frac{1}{2}\left(1 - (-1)^{|S\cap\{a,b\}|}\right) e_{S\oplus\{a,b\}} \\ &= \begin{cases} e_{S\oplus\{a,b\}}, & \text{if } |S\cap\{a,b\}| = 1; \\ 0, & \text{otherwise.}\end{cases}\end{aligned}$$

Using

$$(S \oplus \{a,b\}) \oplus S = \{a,b\},$$

we get that

$$\begin{aligned} H_{XY} e_S &= \frac{1}{2} \sum_{\{a,b\}\in E(G)} \left(\sigma_a^x\sigma_b^x + \sigma_a^y\sigma_b^y\right) e_S \\ &= \sum_{\substack{T\subset V(G) \\ |T|=|S| \\ S\oplus T\in E(G)}} e_T. \end{aligned}$$

The last sum is over the neighbours of S in $G^{\{k\}}$, which completes the proof. □

Notice that $X^{\{1\}} = X$. Thus, when $|S| = 1$, the operation of H_{XY} acting on the subspace spanned by the vectors e_a for $a \in V(G)$, is represented by the adjacency matrix of G.

Similarly, to know the image of e_S under H_{XYZ}, we first need to understand how it acts on a pair of qubits. For an edge $\{a,b\} \in E(G)$, we have that

$$\frac{1}{2}\left(\sigma_a^x\sigma_b^x + \sigma_a^y\sigma_b^y + \sigma_a^z\sigma_b^z\right) e_S = \frac{1}{2}\left(1 - (-1)^{|S\cap\{a,b\}|}\right) e_{S\oplus\{a,b\}} + \frac{1}{2}(-1)^{|S\cap\{a,b\}|} e_S.$$

Then we have that

$$\begin{aligned}
H_{XYZ}e_S &= \frac{1}{2}\sum_{\{a,b\}\in E(G)} \left(\sigma_a^x\sigma_b^x + \sigma_a^y\sigma_b^y + \sigma_a^z\sigma_b^z\right) e_S \\
&= \sum_{\substack{T\subset V(G)\\ |T|=|S| \\ S\oplus T\in E(G)}} e_T + \frac{1}{2}(-1)^{|S\cap\{a,b\}|} e_S \\
&= \sum_{\substack{T\subset V(G)\\ |T|=|S| \\ S\oplus T\in E(G)}} e_T + \frac{1}{2}\left(|E(G)|\, e_S - 2\sum_{\substack{\{a,b\}: \\ |S\cap\{a,b\}|=1}} e_S\right) \\
&= \sum_{\substack{T\subset V(G)\\ |T|=|S| \\ S\oplus T\in E(G)}} e_T + \frac{1}{2}\left(|E(G)|\, e_S - 2\sum_{\substack{T\subset V(G)\\ |T|=|S| \\ S\oplus T\in E(G)}} e_S\right).
\end{aligned}$$

Thus, if $|S| = k$, then H_{XYZ} acting on the span of basis vectors e_S where S is a k-subset of $V(G)$ is represented by

$$A\left(X^{\{k\}}\right) + \frac{1}{2}\,|E(G)|\, I - \Delta\left(X^{\{k\}}\right). \tag{2.2.1}$$

When $k = 1$, in terms of the transition matrix, the expression 2.2.1 is equivalent to the Laplacian $\Delta(G) - A(G)$ of G, up to a constant.

Another reasonable Hamiltonian is $H_{XY\overline{Z}}$. For the Hamiltonian

$$H_{XY\overline{Z}} = \frac{1}{2}\sum_{\{a,b\}\in E(G)} \left(\sigma_a^x\sigma_b^x + \sigma_a^y\sigma_b^y - \sigma_a^z\sigma_b^z\right),$$

by the similar argument as above, we can see that it acting on the subspace spanned by the vectors e_S with S being a k-subsets of $V(G)$ can be represented by the matrix

$$A\left(X^{\{k\}}\right) - \frac{1}{2}\,|E(G)|\, I + \Delta\left(X^{\{k\}}\right).$$

In terms of the transition matrix, this is equivalent to the unsigned Laplacian $A(G) + \Delta(G)$ of G up to a constant.

Therefore, the adjacency matrix and the Laplacian as well as the unsigned Laplacian of a graph are legitimate choices for Hamiltonian of a quantum walk on the graph. Although this thesis will focus on the case when the Laplacian of a graph is used to be Hamiltonian, we will briefly introduce the case when Hamiltonian is the adjacency matrix of a graph, which is also the most investigated case among all three choices.

The most common used definition of a continuous quantum walk on G is the one using the adjacency matrix of G to be Hamiltonian. When a continuous quantum walk on G is generated by $A(G)$, we use vertices to represent quantum states. More specifically, we use the characteristic vector of vertex a in G denoted by $e_a \in \mathbb{R}^n$ to represent a *vertex state* in the quantum walk on G. In the case of vertex state transfer, the transition matrix is

$$U(t) = \exp\left(itA(G)\right).$$

In quantum information processing, one important task is the transfer of quantum states from one location to another location. A system initialized in the state e_a, then at time t, the system is in the state

$$U(t)e_a.$$

As stated before, one rare phenomenon that people care about is perfect state transfer. There is *perfect state transfer* from vertex a to vertex b on G at time τ if and only if

$$\exp\left(i\tau A(G)\right)e_a = \gamma e_b,$$

where γ is a complex unit scalar called the *phase factor* (Lemma 2.5.1). Actually the phase factor associated with perfect state transfer always has norm one. Later on, we will provide a proof in terms of edge state transfer in Lemma 2.5.1 and the same argument holds for vertex state as well.

Another important property of a quantum state is *periodicity*, which can be considered as a special case of perfect state transfer. We say a vertex state e_a is periodic with period τ if

$$\exp\left(i\tau A(G)\right)e_a = \gamma e_a,$$

where γ is a complex scalar.

2.3 Transition Matrices

For a Hermitian matrix H, the transition operator associated with H is

$$U(t) = \exp(itH).$$

A continuous quantum walk is governed by its transition operator $U(t)$. In this section, we introduce some basic properties of transition matrices.

One important property of exponential functions is that if M, N are two matrices that commute with each other, then

$$\exp(M + N) = \exp(M)\exp(N).$$

It follows immediately that

$$U(t_1 + t_2) = U(t_1)U(t_2).$$

A matrix M is *unitary* if

$$MM^* = I.$$

Since H is Hermitian and

$$U(t)^* = \exp(-itH) = U(-t),$$

we see that

$$U(t)U(t)^* = I,$$

which implies that $U(t)$ is unitary.

If the initial state of a system is e_a, then at time t, the probability that the system is in the state e_b is given by

$$e_b^T \left(U(t)e_a \circ \overline{U(t)e_a} \right) = e_b^T \left(U(t) \circ \overline{U(t)} \right) e_a.$$

Since $U(t)$ is unitary, the norm of each row and column is 1. The *mixing matrix* of a continuous quantum walk with transition matrix $U(t)$ is the matrix $M(t)$ such that

$$M(t) = U(t) \circ U(-t),$$

and hence, we know that

$$0 \leq M(t)_{j,k} = \left|U(t)_{j,k}\right|^2 \leq 1.$$

Each column of M represents a probability density. That is, the entry $M(t)_{a,b}$ is the probability that the system is in the state e_b at time t, given that the system initialized in the state e_a. If there is an entry $M(t)_{i,j}$ equal to 1 in the j-th column of M and 0 everywhere else in the column, we know there is perfect state transfer from the state i-th column representing to the state j-th column representing.

2.4 Spectral Decomposition

Algebraic graph theory is the tool used in this thesis to study continuous-time quantum walks. In this section, we build a connection between continuous quantum walks and algebraic graph theory using the spectral decomposition of transition matrices. One can refer to Godsil and Royle [15, Section 8.12] for more details.

Let M be a real symmetric matrix and let $\{\theta_1, \theta_2, \cdots, \theta_n\}$ denote the eigenvalues of M. Then the *spectral decomposition* of M is

$$M = \sum_{i=1}^{n} \theta_i E_i, \tag{2.4.1}$$

where the matrices $E_1, E_2, \cdots, E_n$ satisfy:

(i) $\sum_{i=1}^{n} E_i = I$,

(ii) $E_r E_s = \begin{cases} 0 & \text{if } r \neq s \\ E_r & \text{if } r = s \end{cases}$.

A matrix E is an *idempotent* if $E^2 = E$. The matrices $E_1, E_2, \cdots, E_n$ in Equation 2.4.1 are called *spectral idempotents* and E_r represents the orthogonal projection onto the θ_r-eigenspace of M.

Let $\{v_1, v_2, \cdots, v_k\}$ be orthonormal eigenvectors of M with eigenvalue θ_r with multiplicity k. Then the spectral idempotent E_r of M is uniquely determined by those eigenvectors. That is,

$$E_r = \sum_{i=1}^{k} v_i v_i^T.$$

Since $E_1, E_2, \cdots, E_n$ in the spectral decompositions are idempotents and $E_r E_s = 0$ if $r \neq s$, we get one important property of the spectral decomposition, which is that

$$M^k = \sum_{i=1}^{n} \theta_i^k E_i.$$

It follows that If p is a polynomial, then

$$p(M) = \sum_{i=1}^{n} p(\theta_i) E_i. \tag{2.4.2}$$

We choose p so that it vanishes on all but one of the eigenvalues of M, so it follows from Equation 2.4.1 that the spectral idempotents are polynomials in M. In the proof of Lemma 3.4.1, we specifically construct such polynomials.

Actually we can derive a more general theorem stated as following.

2.4.1 Theorem. *Let M be a real symmetric matrix and let $\sum_{i=1}^{n} \theta_i E_i$ denote the spectral decomposition of M. If $f(x)$ is an analytic function defined on the eigenvalues of M, then*

$$f(M) = \sum_{i=1}^{n} f(\theta_i) E_i.$$

Proof. We know that $M = \sum_{i=1}^{n} \theta_i E_i$, so we have that

$$f(M) = f\left(\sum_{i=1}^{n} \theta_i E_i\right) = \sum_{i=1}^{n} f(\theta_i E_i).$$

Since E_i are spectral idempotents for $i = 1, \cdots, n$, we have that

$$E_i E_i = E_i.$$

For any polynomial p, we have that

$$p(M) = \sum_{i=1}^{n} p(\theta_i) E_i.$$

Thus, we have that

$$f(M) = \sum_{i=1}^{n} f(\theta_i E_i) = \sum_{i=1}^{n} f(\theta_i) E_i$$

for any analytic function $f(x)$. □

Theorem 2.4.1 helps us to obtain the spectral decomposition of the transition matrix $U(t)$, which brings the spectrum into the picture of continuous quantum walk.

2.4.2 Corollary. *Let $U(t)$ be the transition operator associated with a real symmetric matrix M and let $\sum_{i=1}^{n} \theta_i E_i$ denote the spectral decomposition of M. Then*

$$U(t) = \sum_{i=1}^{n} e^{it\theta_i} E_i.$$

Since the spectral idempotents $E_1, E_2, \cdots, E_n$ satisfy that $E_r E_s = 0$ if $r \neq s$, we have that

$$\begin{aligned} U(t) = \exp(itM) &= \sum_{k=0}^{\infty} \frac{(itM)^k}{k!} \\ &= \sum_{k=0}^{\infty} \frac{1}{k!} (it \sum_{i=1}^{n} \theta_i E_i)^k \\ &= \sum_{k=0}^{\infty} \sum_{i=1}^{n} \frac{1}{k!} (it\theta_i)^k E_i \\ &= \sum_{i=1}^{n} e^{it\theta_i} E_i, \end{aligned}$$

which completes our proof. □

2.5 Edge State Transfer

In this section, we introduce another way to define a continuous quantum walk on a graph, that is, using the Laplacian of the graph as Hamiltonian. This is the definition we used in this thesis to study state transfer during quantum communication.

Let G be a graph with n vertices. Let $A(G)$ denote the adjacency matrix of G and let $\Delta(G)$ denote the degree matrix of G . Then the *Laplacian* of G is the matrix $L(G)$ such that

$$L(G) = \Delta(G) - A(G).$$

Instead of using vertices, we can use edges to identify quantum states and in this case, the Laplacian is the Hamiltonian associated to the quantum quantum walk on G. The transition matrix is

$$U(t) = \exp(itL).$$

For example, the spectral decomposition of the Laplacian L of P_3 is

$$L = 0\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} + 1\begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} + 3\begin{pmatrix} \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \end{pmatrix}. \tag{2.5.1}$$

Then by Corollary 2.4.2, the transition matrix associated is

$$U(t) = e^{0it}\begin{pmatrix} \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} + e^{it}\begin{pmatrix} \frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & 0 & 0 \\ -\frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix} + e^{3it}\begin{pmatrix} \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ \frac{1}{6} & -\frac{1}{3} & \frac{1}{6} \end{pmatrix}$$

$$= \begin{pmatrix} \frac{1}{3} + \frac{1}{2}e^{it} + \frac{1}{6}e^{3it} & \frac{1}{3} - \frac{1}{3}e^{3it} & \frac{1}{3} - \frac{1}{2}e^{it} + \frac{1}{6}e^{3it} \\ \frac{1}{3} - \frac{1}{3}e^{3it} & \frac{1}{3} + \frac{2}{3}e^{3it} & \frac{1}{3} - \frac{1}{3}e^{3it} \\ \frac{1}{3} - \frac{1}{2}e^{it} + \frac{1}{6}e^{3it} & \frac{1}{3} - \frac{1}{3}e^{3it} & \frac{1}{3} + \frac{1}{2}e^{it} + \frac{1}{6}e^{3it} \end{pmatrix}$$

A edge (a, b) of G represents the quantum *edge state*

$$e_a - e_b,$$

where $e_a, e_b \in \mathbb{R}^n$ are the characteristic vectors of a, b respectively. We want quantum states to be represented by unit vectors, so when we perform computations about edge state transfer, we use the normalized edge state

$$\frac{1}{\sqrt{2}}(e_a - e_b),$$

but except for that, we always use $e_a - e_b$ to denote our edge states for convenience. Unless explicitly stated otherwise, we use edge states in the continuous quantum walk on G generated by the Laplacian of G.

A system initialized in the state $e_a - e_b$, and at time t, the system is in the state

$$U(t)(e_a - e_b).$$

Perfect state transfer and periodicity are also two important phenomena in quantum edge state transfer. There is *perfect edge state transfer* from edge (a, b) to edge (c, d) at time τ if and only if

$$U(\tau)(e_a - e_b) = \gamma(e_c - e_d),$$

where γ is a complex scalar. In terms of the probability distribution, there is perfect state transfer from $e_a - e_b$ to $e_c - e_d$ at time t if and only if

$$\left|\frac{1}{2}(e_c - e_d)U(t)(e_a - e_b)\right|^2 = 1.$$

When $t = \frac{\pi}{2}$, the transition matrix of P_3 is

$$U\left(\frac{\pi}{2}\right) = \begin{pmatrix} \frac{1}{3}+\frac{1}{3}i & \frac{1}{3}+\frac{1}{3}i & \frac{1}{3}-\frac{2}{3}i \\ \frac{1}{3}+\frac{1}{3}i & \frac{1}{3}-\frac{2}{3}i & \frac{1}{3}+\frac{1}{3}i \\ \frac{1}{3}-\frac{2}{3}i & \frac{1}{3}+\frac{1}{3}i & \frac{1}{3}+\frac{1}{3}i \end{pmatrix}$$

and the mixing matrix is

$$M\left(\frac{\pi}{2}\right) = \begin{pmatrix} \frac{2}{9} & \frac{2}{9} & \frac{5}{9} \\ \frac{2}{9} & \frac{5}{9} & \frac{2}{9} \\ \frac{5}{9} & \frac{2}{9} & \frac{2}{9} \end{pmatrix}.$$

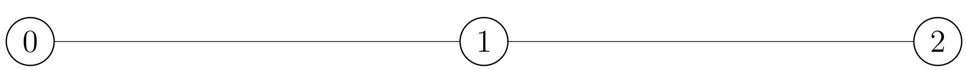

Figure 2.1: P_3

Then we can see that

$$\begin{aligned}\left|\frac{1}{2}(e_1-e_2)U\left(\frac{\pi}{2}\right)(e_0-e_1)\right|^2 &= \left|\frac{1}{2}\left(\frac{1}{3}+\frac{1}{3}i-\left(\frac{1}{3}-\frac{2}{3}i\right)-\left(\frac{1}{3}-\frac{2}{3}i\right)+\frac{1}{3}+\frac{1}{3}i\right)\right|^2\\ &= \left|\frac{1}{2}(2i)\right|^2\\ &= |i|^2\\ &= 1,\end{aligned}$$

which implies that there is perfect edge state transfer from $e_0 - e_1$ to $e_1 - e_2$ at time $\frac{\pi}{2}$ in P_3. Later on Section 5.4, we will prove actually P_3 and P_4 are the only paths that have perfect edge state transfer.

The *edge periodicity* is analogous to the periodicity of a vertex state. We say edge (a, b) is periodic with period τ if

$$U(\tau)(e_a - e_b) = \gamma(e_c - e_d),$$

where γ is a complex scalar and γ is called the phase factor. When $t = \pi$, the mixing matrix of P_3 is

$$M(\pi) = \begin{pmatrix} \frac{1}{9} & \frac{4}{9} & \frac{4}{9} \\ \frac{4}{9} & \frac{1}{9} & \frac{4}{9} \\ \frac{4}{9} & \frac{4}{9} & \frac{1}{9} \end{pmatrix}$$

and from this, we can see that both edge states $e_0 - e_1$ and $e_1 - e_2$ are periodic with period π.

2.5.1 Lemma. *The phase factor associated with perfect state transfer has norm* 1.

Proof. Assume that there is perfect state transfer from $e_a - e_b$ to $e_c - e_d$ at time t. Then we have that

$$U(t)\left(\frac{1}{\sqrt{2}}(e_a - e_b)\right) = \gamma\left(\frac{1}{\sqrt{2}}(e_c - e_d)\right),$$

for some complex scalar γ. Taking norm of both sides of the equation above, we get that

$$\begin{aligned}\left|U(t)\left(\frac{1}{\sqrt{2}}(e_a-e_b)\right)\right| &= \left|\gamma\left(\frac{1}{\sqrt{2}}(e_c-e_d)\right)\right| \\ |U(t)|\left|\frac{1}{\sqrt{2}}(e_a-e_b)\right| &= |\gamma|\left|\frac{1}{\sqrt{2}}(e_c-e_d)\right|.\end{aligned}$$

Since $U(t)$ is unitary and both edge states are unit vectors, it follows that

$$|\gamma| = 1. \qquad \square$$

Periodicity provides a useful tool for the analysis of perfect state transfer. To see that, later on, we will show the connection between periodicity and perfect state transfer in Section 3.1.

From previous section, we know that the transition matrix $U(t)$ can be written in terms of the spectral decomposition of the Laplacian of G. Let $\sum_r \theta_r E_r$ denote the spectral decomposition of L. Quantum state transfer in G is governed by the transition matrix

$$U(t) = \sum_r e^{it\theta_r} E_r. \tag{2.5.2}$$

Notice that when G is a regular graph with valency k, the Laplacian of G is

$$L = kI - A.$$

Thus, the transition matrix is

$$U(t) = \exp\left(it(kI - A)\right) = e^{itk}e^{-itA},$$

which tells us that the continuous quantum walks generated by L and A are equivalent up to a phase factor.

From Equation 2.5.2, we also can see that the Laplacian eigenvalues of G play a large role in the edge state transfer. Let E_r be a spectral idempotent such that

$$E_r(e_a - e_b) = 0.$$

Then we can see that when we talk about the state transfer started in the state $e_a - e_b$, the eigenvalue θ_r and its idempotent E_r contribute nothing to the evolution. The *eigenvalue support* of the state $e_a - e_b$ is the set of Laplacian eigenvalues θ_r such that the corresponding idempotent E_r satisfies

$$E_r(e_a - e_b) \neq 0.$$

Recall the example of P_3 in Section 2.5. From the spectral decomposition 2.5.1 of the Laplacian of P_3, we can see that the eigenvalue supports of edge states $e_0 - e_1$ and $e_1 - e_2$ are the same, that is, $\{1, 3\}$.

Thus, when we talk about quantum state transfer initialized in the state $e_a - e_b$, we only care about the eigenvalues in the eigenvalue support of $e_a - e_b$.

2.6 Eigenvalue Supports

In this section, we study basic properties of the eigenvalue support of an edge state. When we use the adjacency matrix to model continuous quantum walks, we can derive an analogous definition of the eigenvalue support of a vertex state and analogues of all the theorems in this section also hold for the eigenvalue support of a vertex state. But since the main concern of this thesis is edge state transfer, we only provide the definitions and proofs in terms of edge state transfer.

We say two states $e_a - e_b$ and $e_c - e_d$ are *strongly cospectral* in G if and only if for each spectral idempotent E_r of the Laplacian of G, we have

$$E_r(e_a - e_b) = \pm E_r(e_c - e_d).$$

Thus, we can see that if two states are strongly cospectral in graph G, then their eigenvalue supports are the same.

2.6.1 Theorem. *If there is a perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in graph G, then $e_a - e_b$ and $e_c - e_d$ are strongly cospectral.*

Proof. Let $U(t)$ denote the transition matrix associated with G. There is perfect state transfer between $e_a - e_b$ and $e_c - e_d$, which means that

$$U(t)(e_a - e_b) = \gamma(e_c - e_d)$$

for some phase factor γ with $|\gamma| = 1$. Let $\sum_r \theta_r E_r$ denote the spectral decomposition of the Laplacian of G. We see that

$$U(t)(e_a - e_b) = \sum_r e^{it\theta_r} E_r(e_a - e_b) = \gamma(e_c - e_d).$$

By multiplying both sides of the equation above by E_r, we get that

$$e^{it\theta_r}E_r(e_a - e_b) = \gamma E_r(e_c - e_d),$$
$$\gamma^{-1}e^{it\theta_r}E_r(e_a - e_b) = E_r(e_c - e_d).$$

Since both $E_r(e_a - e_b)$ and $E_r(e_c - e_d)$ are real and have the same length, it follows that

$$\gamma^{-1}e^{it\theta_r} = \pm 1,$$

which gives us that

$$E_r(e_a - e_b) = \pm E_r(e_c - e_d).$$

Therefore, $e_a - e_b$ and $e_c - e_d$ are strongly cospectral. □

2.6.2 Corollary. *If there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in G, then $e_a - e_b$ and $e_c - e_d$ have the same eigenvalue support.*

Proof. Let θ_r be an eigenvalue in the eigenvalue support of $e_a - e_b$. Then we have that

$$E_r(e_a - e_b) \neq 0.$$

Since there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$, we know that

$$E_r(e_c - e_d) = \pm E_r(e_a - e_b) \neq 0.$$

Thus, we can conclude that $e_a - e_b$ and $e_c - e_d$ have the same eigenvalue support. □

An *automorphism* of G is an isomorphism from a graph G to itself and the set of all the automorphisms of G form a group, which is called the *automorphism group* of G and denoted by $\mathrm{Aut}(G)$. The following theorem shows that automorphisms also preserve the eigenvalue support of edge states.

2.6.3 Theorem. *Let G be a graph and (a, b) is an edge of G. If there is a permutation $\sigma \in \mathrm{Aut}(G)$ such that $\sigma(e_a - e_b) = e_c - e_d$, then $e_a - e_b$ and $e_c - e_d$ have the same eigenvalue support.*

Proof. Let P denote the permutation matrix associated with $\sigma \in \mathrm{Aut}(G)$. Since $\mathrm{Col}(A)$ is invariant under P, we have that

$$PA = AP.$$

Let Δ denote the degree matrix of G. We know that Δ is a diagonal matrix, so that P commutes with Δ. Let L denote the Laplacian matrix of G. Thus, we have that

$$LP = (\Delta - A)\,P = P\,(\Delta - A) = PL.$$

Let $\sum_r \theta_r E_r$ denote the spectral decomposition of L. Later in the proof of Lemma 3.4.1, we will show that E_r is a polynomial in L and hence, we know that L commutes with E_r. Then we have that

$$PE_r(e_a - e_b) = E_r P(e_a - e_b) = E_r(e_c - e_d).$$

We know that θ_r is not in the eigenvalue support of $e_a - e_b$ if and only if

$$E_r(e_a - e_b) = 0.$$

Since P acts on $E_r(e_a - e_b)$ by permuting its entries, we can see that $E_r(e_a - e_b) = 0$ if and only if

$$PE_r(e_a - e_b) = E_r(e_c - e_d) = 0.$$

Thus, we can conclude that θ_r is not in the eigenvalue support of $e_a - e_b$ if and only if θ_r is not in the eigenvalue support of $e_c - e_d$. □

2.6.4 Corollary. *Let G be an edge-transitive graph. Then all the edge states of G have the same eigenvalue support.* □

2.7 Computational Information

G_n	Total	Adjacency Matrix	Prop.	Laplacian	Prop.
G_5	21	7	33.3%	13	61.9%
G_6	112	10	8.9%	50	44.6%
G_7	853	23	2.7%	191	22.4%
G_8	11117	40	0.4%	1265	11.4%

Table 2.1: Periodic Vertices

Let G_n denote the set of connected graphs on n vertices and the second column shows the cardinality of the corresponding G_n. The third column shows the number of graphs with periodic vertices in G_n when the adjacency matrices are the Hamiltonians and the fourth column shows the corresponding proportion. The fifth column shows the number of graphs with periodic vertices in G_n when the Laplacians are the Hamiltonians and the last column shows the corresponding proportion. One can refer to Godsil's website (`https://www.math.uwaterloo.ca/~cgodsil/agth/projects/pst/period/index.html`) for the details on computing periodic vertices.

G_n	Total	Periodic Edges	Prop.	Edge PST	Prop.
G_5	21	18	85.7%	6	28.6%
G_6	112	86	76.8%	25	22.3%
G_7	853	513	60.1%	94	11.0%
G_8	11117	5164	46.5%	673	6.0%

Table 2.2: Edge State Transfer

Let G_n denote the set of connected graphs on n vertices. The numbers in the third column count the number of graphs with periodic edge states with the Laplacaian being Hamiltonian and the next column shows its proportion. The fifth column shows the number of graphs where there is perfect state transfer and the next column shows the corresponding proportion.

Later on Theorem 3.1.2 tells us that periodicity is necessary condition for a state to have perfect state transfer. Given the rareness of periodic vertices shown in Table 2.1, one cannot expect the perfect state transfer occurs more often than periodic vertices in vertex state transfer. From Table 2.2, we can see that there are more the periodic edges than periodic vertices. This implies the perfect edge state transfer occurs more often than perfect vertex state transfer.

Perfect state transfer is a significant phenomenon in quantum communication but quite rare in quantum walks. We always aim to find more graphs with perfect state transfer. Compared to vertex state transfer with respect to the adjacency matrix, there are more perfect edge state transfer with respect to the Laplacians on the same set of graphs. This is a huge advantage of Laplacian edge state transfer and this is also why the author is interested in Laplacian edge state transfer.

Chapter 3

Earlier Work

In this chapter, we adapt the results from earlier work about vertex state transfer to edge state transfer, and introduce some basic properties of periodicity and perfect state transfer in edge state transfer. Here, we use density matrices to prove the most of our results. Since the results are proved in terms of density matrices, it means that the form of initial states is not restricted. Thus, unless stated explicitly otherwise, the results here work for vertex states, edge states as well as plus states, which we will define later in Chapter 6.

A *density matrix* is a semidefinite matrix of trace 1 and physicists often use a density matrix to represent a quantum state. A density matrix D represents a pure state if $\operatorname{rk} D = 1$. If e_a denotes the standard basis vector in $\mathbb{C}^{V(G)}$ indexed by the vertex a in graph G, then

$$D = \frac{1}{2}(e_a - e_b)(e_a - e_b)^T$$

is a pure state associated with the edge (a, b) in G, which we call the density matrix of edge (a, b). Given a density matrix D as the initial state of a continuous quantum walk, then the state that D is transferred to at time t is given by

$$D(t) = U(t)DU(-t),$$

where $U(t) = \exp(itL)$ is the usual transition matrix associated with G whose Laplacian matrix is L. There is perfect state transfer between density matrices P and Q means that there is a time t such that

$$Q = U(t)PU(-t).$$

We say a state P is periodic if there is a time t such that

$$P = U(t)PU(-t).$$

Since in the proofs in this chapter we only require our states to be real density matrices, i.e., real positive semidefinite matrices with trace one, the results can be extended to density matrices not of the form zz^* for some complex unit vector z. The original results and proofs using vertex state transfer can be found in [13].

3.1 Perfect State Transfer

In this section, we introduce the symmetry and monogamy properties of perfect state transfer. We use the connection between perfect state transfer and periodicity in terms of timing to show the monogamy property of perfect state transfer.

3.1.1 Theorem. *There is perfect state transfer from $e_a - e_b$ to $e_c - e_d$ in graph G at time τ if and only if there is perfect state transfer from $e_c - e_d$ to $e_a - e_b$ at time τ.*

Proof. Let P denote the density matrix of $e_a - e_b$ and Q denote the density matrix of $e_c - e_d$. Let $U(t)$ be the transition matrix associated with G. There is perfect state transfer from P to Q at time τ if and only if $U(\tau)PU(-\tau) = Q$. Since both P and Q are real matrices, taking complex conjugate of $U(\tau)PU(-\tau) = Q$ yields

$$U(-\tau)PU(\tau) = Q.$$

We can get that

$$\begin{aligned} U(\tau)QU(-\tau) &= U(\tau)U(-\tau)PU(\tau)U(-\tau) \\ &= P. \end{aligned}$$

Thus, there is perfect state transfer from P to Q at time τ if and only if there is perfect state transfer from Q to P at τ. □

3.1.2 Theorem. *Suppose that $e_a - e_b$ has perfect state transfer at time τ in graph G. Then $e_a - e_b$ is periodic at time 2τ.*

Proof. Assume there is perfect state transfer from $e_a - e_b$ to $e_c - e_d$ at time τ in G. Let P denote the density matrix of $e_a - e_b$ and Q denote the density matrix of $e_c - e_d$. Let $U(t)$ be the transition matrix associated with G. Then we have that

$$U(\tau)PU(-\tau) = Q.$$

It follows that

$$\begin{aligned} U(2\tau)PU(-2\tau) &= U(\tau)U(\tau)PU(-\tau)U(-\tau) \\ &= U(\tau)QU(-\tau) \\ &= P, \end{aligned}$$

which means that P is periodic at 2τ. □

Now we know that if there is perfect state transfer between two states at time τ, then both states are periodic at 2τ. On the other hand, if we know the period of a state that has perfect state transfer is t, then the perfect state transfer occurs exactly at half of the period, $\frac{1}{2}t$. The monogamy of perfect state transfer follows immediately, which states that if a state has perfect state transfer, there is a unique state it gets transferred to.

3.1.3 Theorem. *If there is perfect state transfer between edge (a, b) and (c, d) in graph G, then both edges (a, b) and (c, d) are periodic with the same minimum period. If the minimum period is σ, then perfect state transfer between the two edges occurs at time $\frac{1}{2}\sigma$.*

Proof. Let P be the density matrix of edge (a, b) and Q be the density matrix of edge (c, d). By the definition of density matrices, we have that

$$P = \frac{1}{2}(e_a - e_b)(e_a - e_b)^T \quad \text{and} \quad Q = \frac{1}{2}(e_c - e_d)(e_c - e_d)^T.$$

Suppose there is perfect state transfer between edge (a, b) and (c, d), which implies that there is some t such that

$$\begin{aligned} U(t)PU(-t) &= Q \\ U(t)QU(-t) &= P. \end{aligned}$$

Then we can have

$$\begin{aligned} U(2t)PU(-2t) &= U(t)U(t)PU(-t)U(-t) \\ &= U(t)QU(-t) \\ &= P. \end{aligned}$$

Thus, P is periodic. Similarly, we can get that Q is periodic.
Now suppose the minimum period of P is σ. Let $T = \{t : U(t)PU(-t) = Q\}$. For any $t \in T$, by the argument above we know that P is periodic at $2t$. Let τ denote the least positive element of T. Since σ is the minimum period of P, then we have

$$\begin{aligned} 2\tau &\geq \sigma \\ \tau &\geq \frac{1}{2}\sigma. \end{aligned}$$

If $\tau > \sigma$, then we have that

$$\begin{aligned} U(\tau - \sigma)PU(\sigma - \tau) &= U(\tau)U(-\sigma)PU(\sigma)U(-\tau) \\ &= U(\tau)U(\sigma)PU(-\sigma)U(-\tau) \\ &= U(\tau)PU(-\tau) \\ &= Q, \end{aligned}$$

which means that $\tau - \sigma \in T$ but this contradicts the assumption that τ is the least positive element in T. Since τ is not a period, $\tau < \sigma$. Since σ must divide 2τ, we have

$$\begin{aligned} m\sigma &= 2\tau \\ \tau &= m \cdot \frac{\sigma}{2} < \sigma \end{aligned}$$

for some positive integer m.

Thus, $m = 1$. Therefore, if the minimum period of P is σ, then perfect state transfer occurs at $\frac{\sigma}{2}$. □

3.1.4 Corollary. *For any edge (a, b), there is at most one edge (c, d) such that there is perfect state transfer from (a, b) to (c, d).*

Proof. Let $P = \frac{1}{2}(e_a - e_b)(e_a - e_b)^T$ denote the density matrix of the edge (a, b). Assume there is perfect state transfer from P and then we know that P is periodic with period, say σ. By the theorem above, we know that the perfect state transfer starting from P must happen at time $\frac{\sigma}{2}$. Thus, the density matrix of the state that P gets transfered to is

$$U\left(\frac{\sigma}{2}\right) PU\left(-\frac{\sigma}{2}\right),$$

which is unique. □

The period of a state involved in perfect state transfer can tell us the exact time when the perfect state transfer occurs. So we would like to explore more about periods of periodic states.

3.2 Characterizing Periodicity

In this section, we give two ways to characterize periodicity of an edge state. One way is using the density matrix of a state and the other is to look at the eigenvalue support of a state.

3.2.1 Theorem (the Ratio Condition)**.** *Let $U(t)$ be the transition matrix corresponding to a graph G. Let $\sum_r \theta_r E_r$ be the spectral decomposition of the Laplacian of G. Then $e_a - e_b$ is periodic in G if and only if*

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_l} \in \mathbb{Q}$$

for any $\theta_r, \theta_s, \theta_l, \theta_s$ in the eigenvalue support of $(e_a - e_b)$ with $\theta_l \neq \theta_k$.

Proof. Let D_{ab} denote the density matrix of $e_a - e_b$. By the definition of periodicity, we know that $e_a - e_b$ is periodic if and only if

$$D_{ab} = U(t) D_{ab} U(-t)$$

for some t. We have that D_{ab} is periodic if and only if

$$\begin{aligned} D_{ab} = U(t) D_{ab} U(-t) &= \sum_{r,s} e^{it(\theta_r - \theta_s)} E_r D_{ab} E_s \\ &= \sum_{r,s} \cos\left(it(\theta_r - \theta_s)\right) E_r D_{ab} E_s \\ &\quad + i \left(\sum_{r,s} \sin\left(it(\theta_r - \theta_s)\right) E_r D_{ab} E_s \right) \end{aligned}$$

Since every entry of D_{ab} is real, we need the imaginary part of $U(t) D_{ab} U(-t)$ to be zero. That is,

$$\sum_{r,s} \sin\left(it(\theta_r - \theta_s)\right) E_r D_{ab} E_s = 0.$$

Since for any two distinct $E_rD_{ab}E_s$'s, we have that

$$\begin{aligned}\langle E_rD_{ab}E_s, E_xD_{ab}E_y\rangle &= \operatorname{tr}(E_rD_{ab}E_s \cdot E_xD_{ab}E_y)\\ &= \operatorname{tr}(D_{ab}E_sE_xD_{ab}E_yE_r)\\ &= 0,\end{aligned}$$

which implies that the non-zero matrices $E_rD_{ab}E_s$'s are linearly independent. Thus, the imaginary part of $U(t)D_{ab}U(-t)$ equals zero if and only if $\sin(it(\theta_r - \theta_s)) = 0$ whenever $E_rD_{ab}E_s \neq 0$. Let S be the eigenvalue support of $(e_a - e_b)$ in G. Then we can conclude that for all eigenvalues $\theta_r, \theta_s \in S$, there is an integer $m_{r,s}$ such that $t(\theta_r - \theta_s) = m_{r,s}\pi$. It follows that for any $\theta_r, \theta_s, \theta_l, \theta_k \in S$ and $\theta_l \neq \theta_k$, we must have

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_l} = \frac{m_{r,s}}{m_{k,l}} \in \mathbb{Q}$$

if and only if $U(t)D_{ab}U(-t)$ is a real matrix.
Since $\sum_r E_r = I$, we can have that $U(t)D_{ab}U(-t)$ is real, i.e.,

$$U(t)D_{ab}U(-t) = \sum_{r,s} \cos(it(\theta_r - \theta_s))\, E_rD_{ab}E_s = I \cdot D_{ab} \cdot I = D_{ab},$$

if and only if the edge $e_a - e_b$ is periodic. □

3.2.2 Corollary. *Let $U(t)$ be the transition matrix corresponding to a graph G. Let $\sum_r \theta_r E_r$ be the spectral decomposition of the Laplacian of G. Then the density matrix D_{ab} of $e_a - e_b$ is real if and only if*

$$\frac{\theta_r - \theta_s}{\theta_k - \theta_l} \in \mathbb{Q}$$

for any $\theta_r, \theta_s, \theta_l, \theta_k$ in the eigenvalue support of $(e_a - e_b)$ and $\theta_l \neq \theta_k$.

Proof. Directly from the proof of previous theorem. □

3.2.3 Corollary. *Let D_{ab} denote the density matrix of $e_a - e_b$. Then D_{ab} is real if and only if $e_a - e_b$ is periodic in graph G.* □

Actually the ratio condition also gives us another way to characterize periodicity. A state is periodic if and only if the eigenvalues in its eigenvalue support are either all integers or the difference of any two eigenvalues in its eigenvalue support is an integer multiple of $\sqrt{\Delta}$ for some square-free integer Δ.

3.2.4 Lemma. *Given a matrix L, if θ is an eigenvalue of L, then its algebraic conjugates are also eigenvalues of L.*

Proof. Let $\{\theta_1, \theta_2, \cdots, \theta_n\}$ denote the algebraic conjugates of θ. Then we know there is an irreducible monic polynomial $f(x)$ such that$\{\theta, \theta_1, \theta_2, \cdots, \theta_n\}$ are roots of $f(x)$. Since θ is an eigenvalue of L, it is a root of the characteristic polynomial of L. By the definition of minimal polynomial, we get $f(x)$ divides the characteristic polynomial of L. Hence, $\{\theta_1, \theta_2, \cdots, \theta_n\}$ are roots of the characteristic polynomial of L as well. □

3.2.5 Lemma. *Let $\sum_r \theta_r E_r$ denote the spectral decomposition of a diagonalizable matrix L. If θ_r and θ_s are algebraic conjugates, then the corresponding spectral idempotents E_r and E_s are also algebraic conjugates.*

Proof. We fix an eigenvalue θ_r and consider a polynomial

$$h_r(x) = \prod_{t \neq r} \frac{x - \theta_t}{\theta_r - \theta_t},$$

which has the properties that $h(\theta_r) = 1$ and $h(\theta_t) = 0$ for all $t \neq r$. Since $L = \sum_r \theta_r E_r$, we can have that

$$h_r(L) = \sum_r h_r(\theta_r) E_r = E_r.$$

Let $\sigma \in \mathrm{Gal}\left(\mathbb{Q}(\theta_r, \theta_s)\right)$ such that $\sigma(\theta_r) = \theta_s$. By applying σ to $h_r(x)$, we can get a new polynomial

$$h_s(x) = \prod_{t \neq s} \frac{x - \theta_t}{\theta_s - \theta_t}.$$

Then we have that

$$h_s\left(L\right) = E_s.$$

We can see that $\sigma\left(h_r(L)\right) = h_s(L) = E_s$. Thus, E_r and E_s are algebraic conjugates. □

3.2.6 Lemma. *Given graph G with Laplacian L, let (a, b) be an edge of G with eigenvalue support S. Then if θ is in S, then all its algebraic conjugates will also be in S.*

Proof. Let θ_s be an algebraic conjugate of θ_r. By Lemma 3.2.5, We know that E_r and E_s are algebraic conjugates. Let $f(x)$ be the characteristic polynomial of L and let K be the splitting filed of $f(x)$ over $\mathbb{Q}$. Then there is a element σ in $\mathrm{Gal}(K\backslash\mathbb{Q})$ such that $\sigma(E_r) = E_s$. If $E_r(e_a - e_b) = 0$, we get that

$$\sigma(E_r(e_a - e_b)) = E_s(e_a - e_b) = 0,$$

since all the entries of $e_a - e_b$ are rational. Similarly, if $E_s(e_a - e_b) = 0$, then

$$\sigma^{-1}(E_s(e_a - e_b)) = E_r(e_a - e_b) = 0.$$

Therefore, if θ_r is in the eigenvalue support of $(e_a - e_b)$, then all its algebraic conjugates are also in the eigenvalue support. □

The following theorem can be viewed as a corollary of the ratio condition. Notice that the size of the eigenvalue support of a vertex state in a connected graph with at least two vertices must be at least two while the eigenvalue support of an edge state can have size one. The case when the eigenvalue support of size one can be excluded using a theorem the author proved in the latter chapter and the rest of the proof can be found in Coutinho and Godsil [8] stated in terms of vertex states.

3.2.7 Theorem. *Let G be a graph with the Laplacian matrix L and let (a, b) be an edge of G with eigenvalue support S. Then $e_a - e_b$ is periodic in G if and only if either:*

(i) All the eigenvalues in S are integers;

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

Proof. Assume all the eigenvalues in S satisfy either of the conditions stated above, then by the ratio condition, it is easy to see that (a, b) is a periodic edge.
Assume $e_a - e_b$ is periodic in G. We have already proved that if $|S| = 1$, then (a, b) is periodic in Theorem 5.1.3. Also, if $|S| = 2$, then by Lemma 3.2.6,

the two eigenvalues are either both integers or roots of a quadratic polynomial. Again by the ratio condition, we can say that if $|S| = 2$, then $e_a - e_b$ is periodic. Hence, we assume that $|S| \geq 3$.

Let θ_0 and θ_1 be two distinct eigenvalues in S. We want to show that $(\theta_0 - \theta_1)^2$ is an integer. By the ratio condition, we know that for any $\theta_r, \theta_s \in S$, there is a rational number $a_{r,s}$ such that

$$\theta_r - \theta_s = a_{r,s}(\theta_0 - \theta_1)$$

and hence, we have that

$$\prod_{r \neq s}(\theta_r - \theta_s) = (\theta_0 - \theta_1)^{\binom{|S|}{2}} \prod_{r \neq s} a_{r,s}.$$

Let K denote the splitting field of the characteristic polynomial of G over $\mathbb{Q}$. Then we can see that the left hand side of the equation above is fixed by $\mathrm{Gal}(K \backslash \mathbb{Q})$, which implies that the left is in $\mathbb{Q}$. Since every eigenvalue is an algebraic integer, the left hand side is an integer. Because $a_{r,s}$ is rational for all r, s with $r \neq s$, we get that

$$(\theta_0 - \theta_1)^{\binom{|S|}{2}} \in \mathbb{Q}.$$

Since $(\theta_0 - \theta_1)$ is an algebraic integer, this implies that

$$(\theta_0 - \theta_1)^{\binom{|S|}{2}} \in \mathbb{Z}.$$

Now, let m be the least positive integer such that $(\theta_0 - \theta_1)^m$ is an integer, say β. That is,

$$(\theta_0 - \theta_1)^m = \beta^m$$
$$\theta_0 - \theta_1 = \beta e^{\frac{2\pi i k}{m}} \text{ for } k = 0, 1, \cdots, m-1.$$

But since L is positive semidefinite, all its eigenvalues are real. Thus, we can conclude that $m \leq 2$, which means that $\theta_0 - \theta_1$ is either an integer or a square root of an integer. We have that

$$(\theta_r - \theta_s)^2 = a_{r,s}^2(\theta_0 - \theta_1)^2,$$

where both $a_{r,s}$ and $(\theta_0 - \theta_1)^2$ are rational, then it follows that $(\theta_r - \theta_s)^2$ is rational and hence, it is an integer. So $\theta_r - \theta_s$ is in the form

$$\alpha\sqrt{\Delta_{r,s}}$$

for some $\alpha, \Delta_{r,s} \in \mathbb{Z}$. For $\theta_k, \theta_l \in S$, we have

$$\theta_k - \theta_l = a_{k,l}(\theta_0 - \theta_1)$$

and hence,

$$(\theta_r - \theta_s)(\theta_k - \theta_l) = a_{r,s}a_{k,l}(\theta_0 - \theta_1)^2.$$

Since the right hand side is rational, we know that $(\theta_r - \theta_s)(\theta_k - \theta_l)$ is rational and hence, it is an integer. This implies that $\Delta_{r,s} = \Delta_{k,l}$. Thus, there is a square-free integer Δ and an integer m_r such that for each r, we have

$$\theta_r = \theta_0 - m_r\sqrt{\Delta}.$$

If we sum over all the eigenvalues in S, we get that

$$|S|\,\theta_0 - \sqrt{\Delta}\sum_r m_r = \sum_r \theta_r.$$

We know that $\sum_r \theta_r$ is fixed by $\mathrm{Gal}(K\backslash\mathbb{Q})$, so $\sum_r \theta_r$ is rational and hence an integer. Therefore, $\theta_0 \in \mathbb{Q}(\sqrt{\Delta})$. □

3.2.8 Corollary. *If $e_a - e_b$ is periodic in graph G, then any two distinct eigenvalues in the eigenvalue supports of $e_a - e_b$ differ by at least one.*

Proof. Assume that $e_a - e_b$ is periodic in graph G. Let θ_r and θ_s be two distinct eigenvalues in the eigenvalue support of $e_a - e_b$. We know that $\theta_r - \theta_s$ is an integer multiple of $\sqrt{\Delta}$ for some square-free integer Δ. Since $\sqrt{\Delta} \geq \sqrt{2}$, we have that

$$|\theta_r - \theta_s| \geq \sqrt{\Delta} \geq 1,$$

which completes our proof. □

3.3 Period

Actually Theorem 3.2.7 allows us to bound the period of a periodic state. This section shows one general bound on the period of a periodic state and a more tight bound on the period under certain condition.

3.3.1 Corollary. *If an edge is periodic in graph G with period τ, then $\tau \leq 2\pi$.*

Proof. Suppose edge (a, b) is periodic in G. Let D_{ab} denote the density matrix of (a, b) and let S denote the eigenvalue support of (a, b). If all the elements in S are integers then

$$\begin{aligned} U(-2\pi)D_{ab}U(2\pi) &= \sum_{r,s} e^{i2\pi(\theta_r - \theta_s)} E_r D_{ab} E_s \\ &= \sum_{r,s} \cos\left(i2\pi(\theta_r - \theta_s)\right) E_r D_{ab} E_s \\ &+ i\left(\sum_{r,s} \sin\left(i2\pi(\theta_r - \theta_s)\right) E_r D_{ab} E_s\right) \\ &= \sum_{r,s} E_r D_{ab} E_s \\ &= D_{ab} \end{aligned}$$

If there is a non-integer element in S, by Theorem 3.2.7, we know that for all θ_r, θ_s in S, the difference $\theta_r - \theta_s$ is an integer multiple of $\sqrt{\Delta}$ for some square-free integer Δ. Then similarly,

$$U(-2\pi/\sqrt{\Delta})\, D_{ab}\, U(2\pi/\sqrt{\Delta}) = D_{ab}$$

Hence, the period of D_{ab} is at most 2π. □

When two density matrices involved in perfect state transfer are trace-orthogonal, we actually can derive a lower bound on the time when perfect state transfer occurs.

3.3.2 Lemma. *Let P denote the density matrix of $e_a - e_b$ and Q denote the density matrix of $e_c - e_d$. Suppose that there is perfect state transfer from P to Q at time t in graph G and that $\theta_1, \theta_2, \cdots, \theta_m$ are the distinct* *eigenvalues of the Laplacian L of G in non-increasing order. If* $\operatorname{tr}(PQ) = 0$, *then*

$$t \geq \frac{\pi}{\theta_1 - \theta_m}.$$

Proof. By the definition of density matrices, P is positive semidefinite, which implies that P has a unique positive semidefinite square root. Let $P^{\frac{1}{2}}$ denote the square root of P. Since $U(t)PU(-t) = Q$, we have that

$$\begin{aligned}
\operatorname{tr}(PQ) &= \operatorname{tr}\left(PU(t)PU(-t)\right) \\
&= \operatorname{tr}\left(P^{\frac{1}{2}}P^{\frac{1}{2}}U(t)P^{\frac{1}{2}}P^{\frac{1}{2}}U(-t)\right) \\
&= \operatorname{tr}\left(P^{\frac{1}{2}}U(t)P^{\frac{1}{2}}P^{\frac{1}{2}}U(-t)P^{\frac{1}{2}}\right) \\
&= \operatorname{tr}\left(\left(P^{\frac{1}{2}}U(t)P^{\frac{1}{2}}\right)\left(P^{\frac{1}{2}}U(t)P^{\frac{1}{2}}\right)^*\right).
\end{aligned}$$

It follows that $\operatorname{tr}(PQ) = 0$ if and only if

$$P^{\frac{1}{2}}U(t)P^{\frac{1}{2}} = 0.$$

Let $\sum_r \theta_r E_r$ be the spectral decomposition of L. Then we have that

$$\begin{aligned}
\operatorname{tr}\left(P^{\frac{1}{2}}U(t)P^{\frac{1}{2}}\right) &= \operatorname{tr}\left(P^{\frac{1}{2}}\sum_r e^{it\theta_r}E_rP^{\frac{1}{2}}\right) \\
&= \sum_r e^{it\theta_r}\operatorname{tr}\left(P^{\frac{1}{2}}E_rP^{\frac{1}{2}}\right).
\end{aligned}$$

Since $P^{\frac{1}{2}}$ and E_r's are positive semidefinite for all r, $P^{\frac{1}{2}}E_rP^{\frac{1}{2}}$'s are positive semidefinite for all r. Thus, we know that for all r, $\operatorname{tr}\left(P^{\frac{1}{2}}E_rP^{\frac{1}{2}}\right) \geq 0$. Also, we have that

$$\sum_r \operatorname{tr}\left(P^{\frac{1}{2}}E_rP^{\frac{1}{2}}\right) = \operatorname{tr}(P) = 1.$$

Hence, if $\operatorname{tr}(PQ) = 0$, by the argument above, we know that we can consider $\operatorname{tr}\left(P^{\frac{1}{2}}U(t)P^{\frac{1}{2}}\right) = 0$ as a convex combination of the eigenvalues of $U(t)$. We can view the eigenvalues of $U(t)$ as being contained in an arc on the unit circle in the complex plane. Since 0 is a convex combination of the eigenvalues, the eigenvalues of $U(t)$ cannot lie on an arc of the unit circle with length less than π. Therefore, we must have

$$t(\theta_1 - \theta_m) \geq \pi,$$

which gives us

$$t \geq \frac{\pi}{\theta_1 - \theta_m}.$$

□

The author adapts the above result that is proven originally by Godsil [14] to edge state transfer and gets a more precise restriction on states when we can use the period bound above. In the case when perfect edge state transfer occurs, if two edges have one vertex in common, we have the lower bound on the time when perfect edge state transfer occurs.

3.3.3 Lemma. *Let P denote the density matrix of edge (a,b) and Q denote the density matrix of edge (c,d). Then edges (a,b) and (c,d) have no vertex in common if and only if $PQ = 0$.*

Proof. We know that

$$P = \frac{1}{2}(e_a - e_b)(e_a - e_b)^T \quad \text{and} \quad Q = \frac{1}{2}(e_c - e_d)(e_c - e_d)^T.$$

Then we have that

$$PQ = \frac{1}{4}(e_a - e_b)\left((e_a - e_b)^T(e_c - e_d)\right)(e_c - e_d)^T.$$

It is easy to see that $(e_a - e_b)^T(e_c - e_d) = 0$ if and only if edges (a,b) and (c,d) have no vertex in common. □

3.3.4 Corollary. *Suppose that there is perfect state transfer between two edges that have one vertex in common at time t in graph G and that $\theta_1, \theta_2, \cdots, \theta_m$ are the distinct eigenvalues of the Laplacian L of G in non-increasing order. Then we have that*

$$t \geq \frac{\pi}{\theta_1 - \theta_m}.$$

□

3.4 Algebra

Let G be a graph with the Laplacian matrix L and (a, b) be an edge of G with density matrix D_{ab}. Given that (a, b) has perfect state transfer in G, we can gain more information about the matrix algebra generated by L and D_{ab}. Automorphisms of G can provide us more edges in G that have perfect state transfer.

3.4.1 Lemma. *Let $U(t)$ be the transition matrix associated with graph G and L denote the Laplacian matrix of G. Then $U(t)$ is a polynomial in L.*

Proof. Let $\sum_m \theta_m E_m$ denote the spectral decomposition of L. Now fix an eigenvalue θ_r of L and define a polynomial $h_r(x)$ such that

$$h_r(x) = \prod_{s \neq r} \frac{x - \theta_s}{\theta_r - \theta_s}.$$

We can see that $h_r(\theta_u) = 0$ for all $u \neq r$ and $h_r(\theta_r) = 1$. We apply $h_r(x)$ to L and then we can get that

$$h_r(L) = \sum_m h_r(\theta_m) E_m = E_m.$$

Thus, for each spectral idempotent E_r of L, E_r is a polynomial in L. Since $U(t)$ is a linear combination of the spectral idempotents of L, $U(t)$ is a polynomial in L. □

3.4.2 Theorem. *Let P denote the density matrix of an edge in graph G and $U(t)$ be the transition matrix associated with G. Define $P(t)$ to be $P(t) = U(t)PU(-t)$. Then the algebra generated by $P(t)$ and L is the same as the algebra generated by P and L. That is,*

$$\langle P(t), L \rangle = \langle P, L \rangle.$$

Proof. By Lemma 3.4.1, we can have that for any t, $U(t)$ is a polynomial in L. So $P(t) \in \langle P, L \rangle$ for all t. Also, we have that $U(-t)P(t)U(t) = P$. Therefore,

$$\langle P(t), L \rangle = \langle P, L \rangle.$$

□

3.4.3 Corollary. *Let P and Q denote two distinct edge states in graph G. If there is perfect state transfer between P and Q, then*

$$\langle P, L\rangle = \langle Q, L\rangle.$$

Proof. Assume that there is perfect state transfer between P and Q at time τ. By Theorem 3.4.2, we know that

$$\langle P(t), L\rangle = \langle P, L\rangle$$

for all t. Then we have

$$\langle Q, L\rangle = \langle U(\tau)PU(-\tau), L\rangle = \langle P, L\rangle.$$

□

As show above, perfect state transfer between edges states in a graph can help us to gain more information about the underlying algebra of the graph. On the other hand, the underlying algebra of a graph can also help us to explore more about perfect state transfer in the graph.

3.4.4 Lemma. *If a graph G admits perfect state transfer between $e_a - e_b$ to $e_c - e_d$, then the stabilizer of $e_a - e_b$ is the same as the stabilizer of $e_c - e_d$ in* $\mathrm{Aut}(G)$*.*

Proof. Let A denote the adjacency matrix of G. We use permutation matrices to identify the automorphisms of G. Since the column space of A is invariant under those permutation matrices associated with automorphisms of G, we know that the permutation matrices commute with A. Let P denote a permutation matrix that associate with some $\sigma \in \mathrm{Aut}(G)$. Since the degree matrix Δ of G is a diagonal matrix, we have that $\Delta P = P\Delta$. Let L denote the Laplacian of G and we know that $L = \Delta - A$. Thus, we have that

$$LP = PL.$$

Since the transition matrix $U(t)$ is $\exp(itL)$, any permutation matrix from $\mathrm{Aut}(G)$ commutes with $U(t)$. Now assume that $P(e_a - e_b) = e_a - e_b$ and $U(\tau)(e_a - e_b) = \gamma(e_c - e_d)$ for some $|\gamma| = 1$. Then we have that

$$\begin{aligned} PU(\tau)(e_a - e_b) &= \gamma P(e_c - e_d) \\ U(\tau)P(e_a - e_b) &= \gamma P(e_c - e_d) \\ \gamma(e_c - e_d) &= \gamma P(e_c - e_d). \end{aligned}$$

Thus, $e_c - e_d$ is also fixed by P. □

The following lemma the author proved can be seen as a corollary of the above lemma proved by Godsil in [13].

3.4.5 Lemma. *If graph G admits perfect state transfer between $e_a - e_b$ to $e_c - e_d$, then all the edge states in the orbit of $e_a - e_b$ under* $\mathrm{Aut}(G)$ *have perfect state transfer.*

Proof. Assume there exist time τ such that $U(\tau)(e_a - e_b) = \gamma(e_c - e_d)$ for some $|\gamma| = 1$. Let P denote a permutation matrix associated with a $\sigma \in \mathrm{Aut}(G)$ and $P(e_a - e_b) = e_{a'} - e_{b'}$. By Lemma 3.4.4, we know P does not fix $(e_c - e_d)$ and assume $P(e_c - e_d) = e_{c'} - e_{d'}$. Then we have

$$\begin{aligned} U(\tau)P(e_a - e_b) &= \gamma P(e_c - e_d) \\ U(\tau)(e_{a'} - e_{b'}) &= \gamma(e_{c'} - e_{d'}). \end{aligned}$$

Thus, there is also perfect state transfer between $e_{a'} - e_{b'}$ and $e_{c'} - e_{d'}$ at time τ. □

By the monogamy of perfect state transfer, the following results follow immediately.

3.4.6 Corollary. *If there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in graph G, then the orbit of $e_a - e_b$ and the orbit of $e_c - e_d$ under* $\mathrm{Aut}(G)$ *must have the same size.* □

3.4.7 Corollary. *Given an edge-transitive graph G, if perfect edge state transfer occurs in G, then all the edges have perfect state transfer.* □

By monogamy property of perfect state transfer, we know that perfect state edge transfer in an edge-transitive graph partition edges into pairs.

3.4.8 Corollary. *Let G be an edge-transitive graph with n edges. If n is odd, there is no edge perfect state transfer in G.*

3.4.9 Corollary. *Given an edge-transitive graph G, if there is a edge that is periodic in G, then all the edges in G are periodic.* □

3.5 Summary

Let P, Q be two distinct edge states. There is perfect state transfer from P to Q in graph G at time τ if and only if there is perfect state transfer from Q to P at the same time. If P has perfect state transfer, then it is periodic and perfect state transfer occurs at exactly half of the period. There is at most one state such that there is perfect state transfer between it and P. Symmetry and monogamy are two basic properties of perfect state transfer.

A state is periodic if and only if the density matrix of the state is real. Periodicity of a state also can be characterized by the ratio condition, which implies that either all the eigenvalues in the eigenvalues support are integers or the difference of any two eigenvalues in the eigenvalue support is an integer multiple of $\sqrt{\Delta}$ for some square-free integer Δ. The characterization using eigenvalues actually helps us to bound the period of a periodic state.

The period of a periodic state is at most 2π and if there is perfect state transfer between P and Q and they are trace-orthogonal, then they have periods at most $\pi / (\theta_1 - \theta_m)$ where θ_1, θ_m are the largest and smallest eigenvalues in the eigenvalue support of P respectively. The bound on the period of a periodic state gives us a bound on the timing when perfect state transfer can occur.

If there is perfect state transfer between P and Q in graph G, then the algebra generated by P and the Laplacian of G is the same as the algebra generated by Q and the Laplcian of G. All the edges in the orbit of a state with perfect state transfer under automorphisms of G also have perfect state transfer. Given a pair of edges involved in perfect state transfer, automorphisms of a graph provides us an efficient way to find more edges with perfect state transfer.

In the next chapter, we use the results of this chapter to explore more about periodicity and perfect state transfer in the case of edge state transfer.

Chapter 4

Constructions and Phenomena

In this chapter, we introduce two ways to build a new graph with perfect state transfer based on some given graphs with perfect state transfer. Also, we introduce the transitivity phenomenon. That is, if there is perfect state transfer from $e_a - e_b$ to $e_\alpha - e_\beta$ and also from $e_b - e_c$ to $e_\beta - e_\gamma$ at the same time t, then there is perfect state transfer from $e_a - e_c$ to $e_\alpha - e_\gamma$ at time t.

4.1 Complement Graph

In this section, we show that given a graph admitting perfect edge state transfer, how to construct a new graph with perfect edge state transfer using the complement of the given graph. Throughout this section, if G is a graph, then $\overline{G}$ denotes the complement of G.

First, we would like to explore the relation between perfect edge state transfer in a graph and in its complement.

4.1.1 Lemma. *Let G be a graph with n vertices and L denote the Laplacian matrix of G. Then every Laplacian eigenvector of G with non-zero eigenvalue θ is a Laplacian eigenvector of $\overline{G}$ with eigenvalue $n - \theta$.*

Proof. Let x denote an eigenvector of L with eigenvalue θ, which means that

$$Lx = \theta x.$$

Let J denote the all-ones matrix. Since all the eigenvectors are orthogonal to each other and the all-ones vector $\mathbf{1}$ is always a Laplacian eigenvector with eigenvalue 0, for any Laplacian eigenvector x with non-zero eigenvalue, we have that $Jx = \mathbf{0}$. Let $\overline{L}$ denote the Laplacian matrix of $\overline{G}$ and then we have that

$$\begin{aligned}\overline{L}x &= (nI - J - L)x \\ &= nx - \mathbf{0} - \theta x \\ &= (n-\theta)x\end{aligned}$$

Therefore, every Laplacian eigenvector of G with non-zero eigenvalue θ is a Laplacian eigenvector of $\overline{G}$ with eigenvalue $n - \theta$. □

Since zero is always an eigenvalue of the Laplacian matrix of a graph with spectral idempotent being the all-ones matrix, we know that a matrix is a Laplacian spectral idempotent of a graph G if and only if it is a Laplacian spectral idempotent of $\overline{G}$.

4.1.2 Theorem. *There is perfect state transfer between $(e_a - e_b)$ and $(e_c - e_d)$ in graph G if and only if there is perfect state transfer between $(e_a - e_b)$ and $(e_c - e_d)$ in $\overline{G}$.*

Proof. Let $S = \{\theta_1, \theta_2, \cdots, \theta_r\}$ denote the eigenvalue support of $(e_a - e_b)$ and $(e_c - e_d)$ in G and $\sum_r \theta_r E_r$ denote the spectral decomposition of the Laplacian of G. Let

$$a_j = (E_j)_{ac} + (E_j)_{ad} - (E_j)_{bc} + (E_j)_{bd}$$

for all eigenvalue $\theta_j \in S$. Then we have that

$$\begin{aligned}\left|\frac{1}{2}(e_c - e_d)^T U(t)(e_a - e_b)\right|^2 &= \left|\frac{1}{2}\sum_{j=1}^{r} e^{it\theta_j}\left((E_j)_{ac} + (E_j)_{ad} - (E_j)_{bc} + (E_j)_{bd}\right)\right|^2 \\ &= \left|\frac{1}{2}\left(a_1 e^{it\theta_1} + a_2 e^{it\theta_2} + \cdots + a_r e^{it\theta_r}\right)\right|^2 \\ &= \frac{1}{4}\big(\,(a_1\cos(\theta_1 t) + a_2\cos(\theta_2 t) + \cdots + a_r\cos(\theta_r t))^2 \\ &+ (a_1\sin(\theta_1 t) + a_2\sin(\theta_2 t) + \cdots + a_r\sin(\theta_r t))^2\,\big) \\ &= \frac{1}{4}\left(a_1^2 + a_2^2 + \cdots + a_r^2 + \sum_{r\neq s} 2a_r a_s\cos((\theta_r - \theta_s)t)\right)\end{aligned}$$

By Lemma 4.1.1, we know that the eigenvalue support $\overline{S}$ of $(e_a - e_b)$ and $(e_c - e_d)$ in $\overline{G}$ is $\{n-\theta_1, n-\theta_2, \cdots, n-\theta_r\}$. Since zero is never in the eigenvalue support, the spectral idempotent $\overline{E_r}$ of $\overline{L}$ with eigenvalue $n-\theta_r$ is the same as E_r with eigenvalue θ_r of L for all eigenvalues in the eigenvalue support of $e_a - e_b$ in G. Let $\overline{U}(t) = \exp(it\overline{L})$ be the transition matrix associated with $\overline{G}$. We have that

$$\begin{aligned}
&\left|\frac{1}{2}(e_c - e_d)^T\overline{U}(t)(e_a - e_b)\right|^2 \\
&= \left|\frac{1}{2}\sum_{j=1}^{r} e^{it(n-\theta_j)}\left((E_j)_{ac} + (E_j)_{ad} - (E_j)_{bc} + (E_j)_{bd}\right)\right|^2 \\
&= \frac{1}{4}\left(a_1^2 + a_2^2 + \cdots + a_r^2 + \sum_{r\neq s} 2a_r a_s \cos\left((n-\theta_r)t - (n-\theta_s)t\right)\right) \\
&= \frac{1}{4}\left(a_1^2 + a_2^2 + \cdots + a_r^2 + \sum_{r\neq s} 2a_r a_s \cos\left((\theta_s-\theta_r)t\right)\right)
\end{aligned}$$

Since cosine is an even function, we get that

$$\left|\frac{1}{2}(e_c - e_d)^T\overline{U}(t)(e_a - e_b)\right|^2 = \left|\frac{1}{2}(e_c - e_d)^T U(t)(e_a - e_b)\right|^2.$$

Therefore, there is perfect state transfer between $(e_a - e_b)$ and $(e_c - e_d)$ in graph G if and only if there is perfect state transfer between them in the complement of G. □

This theorem allows us to build a new graph with perfect edge state transfer based on a graph with perfect edge state transfer. For example, joining a graph with perfect edge state transfer with any other graph will give us a graph with perfect edge state transfer.

Let G_1, G_2 be two graphs. Let E' denote the set of all the edges with one end in $V(G_1)$ and the other end in $V(G_2)$. The *join graph* of G_1 and G_2 is a graph G such that

$$V(G) = V(G_1) \cup V(G_2), E(G) = E(G_1) \cup E(G_2) \cup E'.$$

and the with vertex set $V(G_)$.

4.1.3 Corollary. *Let G be a graph and a, b, c, d are vertices in G. There is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in G if and only if there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in the join graph of G and H for a graph H.*

Proof. Assume that there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in a connected graph G. Let H be a graph with vertex set $V(H)$. Let K denote the join graph of G and H. By Theorem 4.1.2, there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in K if and only if there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in $\overline{K}$.

By the construction of the join graph, we know that all the vertices in $V(G)$ are connected to all the vertices in $V(H)$ in K. So we can see that $\overline{K}$ is a disconnected graph consists of $\overline{G}$ and $\overline{H}$. We know that vertices $a, b, c, d \in V(\overline{G})$. Thus, there is perfect state transfer between$e_a - e_b$ and $e_c - e_d$ in $\overline{K}$ if and only if there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in $\overline{G}$.

The submatrix of the Laplacian matrix of $\overline{K}$ induced by $V(G)$ is the Laplacian matrix of $\overline{G}$. Then we consider the complement of $\overline{G}$, which is G. Again, by Theorem 4.1.2, there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in $\overline{G}$ if and only if there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in G, which completes the proof. □

Let H be a simple graph with one vertex. For a graph G, the join graph of G and H is a cone graph G. So we can see that if there is perfect edge state transfer in a graph G, using Theorem 4.1.2, we can easily construct a cone graph of G to obtain a new graph that admits perfect edge state transfer.

Theorem 4.1.2 also allows us to characterize perfect state transfer in some graphs with special structures.

4.1.4 Corollary. *Let K_n be a complete graph on n vertices and $V(K_n) = \{v_1, v_2, \cdots, v_n\}$. Let G denote the graph obtained from K_n by deleting edge (v_1, v_2). Then there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ for all $i \in \{3, 4, \cdots, n\}$.*

Proof. We know that $\overline{G}$ consists of $n-2$ isolated vertices $\{v_2, v_4, \cdots, v_n\}$ and one edge (v_1, v_2). Let v_i denote an isolated vertex in $\overline{G}$. Let K denote the induced subgraph of $\overline{G}$ by vertices $\{v_1, v_2, v_i\}$. Then we know that $\overline{K}$ is a path on three vertices with v_1, v_2 being two leaves. By Theorem 5.4.7, we know that there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ in $\overline{K}$. Then Theorem 4.1.2 tells us that there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ in K and since (v_1, v_2) is the only edge in $\overline{G}$, there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ in $\overline{G}$. Again Theorem 4.1.2

gives us that there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ in G, which completes our proof. □

4.2 Cartesian Product of Two Graphs

Taking the Cartesian product of two graphs with perfect edge state transfer also can be a method to create a new graph with perfect edge state transfer.

If G, H are two graphs, their *Cartesian product* $G \square H$ has vertex set $V(G) \times V(H)$, where (g_1, h_1) is adjacent to (g_2, h_2) if and only if either

(i) $g_1 = g_2$ in G and h_1 is adjacent to h_2 in H, or

(ii) g_1 is adjacent to g_2 in G and $h_1 = h_2$ in H.

First, we want to explore the connection between the transition matrices of G, H and the transition matrix of $G \square H$.

4.2.1 Lemma. *Let G, H be graphs with Laplacian matrices L_G of order $n \times n$, L_H of order $m \times m$ respectively. Let $G \square H$ denote the Cartesian product of G and H with the Laplacian matrix $L_{G \square H}$. Then $L_{G \square H} = L_G \otimes I + I \otimes L_H$.*

Proof. Let D_G, D_H denote the degree matrix for G and H respectively. We know that $L_G = D_G - A_G$ and $L_H = D_H - A_H$. Since

$$A_{G \square H} = A_G \otimes I_m + I_n \otimes A_H,$$

we have that

$$\begin{aligned} L_{G \square H} &= D_{G \square H} - A_{G \square H} \\ &= (D_G \otimes I_m + I_n \otimes D_H) - (A_G \otimes I_m + I_n \otimes A_H) \\ &= (D_G - A_G) \otimes I_m + I_n \otimes (D_H - A_H) \\ &= L_G \otimes I + I \otimes L_H. \end{aligned}$$

□

4.2.2 Lemma. *Let G, H be two graphs with transition matrices $U_G(t) = \exp(itL_G)$ and $U_H(t) = \exp(itL_H)$ respectively. Let $U_{G \square H}(t) = \exp(itL_{G \square H})$ denote the transition matrix of $G \square H$. Then $U_{G \square H}(t) = U_G(t) \otimes U_H(t)$.*

Proof. Let L_G be a matrix of order $n \times n$ and let L_H be a matrix of order $m \times m$. If M is a matrix of order m and N is a matrix of order $n \times n$, the Kronecker sum of M and N is

$$M \oplus N = M \otimes I_n + I_m \otimes N.$$

Using the Kronecker sum and previous lemma, we have

$$\begin{aligned} U_{G\square H}(t) &= \exp(itL_{G\square H}) \\ &= \exp\left(it(L_G \otimes I_m + I_n \otimes L_H)\right) \\ &= \exp\left(it(L_G \oplus L_H)\right) \\ &= \exp(itL_G) \otimes \exp(itL_H) \\ &= U_G(t) \otimes U_H(t). \end{aligned}$$

□

4.2.3 Theorem. *Let G, H be two graphs, let a, b be two vertices in G and let $\alpha, \beta, \gamma, \kappa$ be vertices in H. There is perfect state transfer between the edge $\{(a,\alpha),(a,\beta)\}$ and the edge $\{(b,\gamma),(b,\kappa)\}$ in $G\square H$ at time t if and only if both of the following conditions hold:*

(i) there is perfect Laplacian vertex state transfer between vertices a and b in G at time t,

(ii) there is perfect edge state transfer between edges (α,β) and (γ,κ) in H at time t.

Proof. The state that denotes the edge $\{(a,\alpha),(a,\beta)\}$ is

$$\frac{1}{\sqrt{2}}(e_a \otimes (e_\alpha - e_\beta))$$

and then we can see that the density matrix of this edge is

$$D_a \otimes D_{\alpha\beta}.$$

Similarly, the density matrix of the edge $\{(b,\gamma),(b,\kappa)\}$ is $D_b \otimes D_{\gamma\kappa}$. There is perfect state transfer between edge $\{(a,\alpha),(a,\beta)\}$ and edge $\{(b,\gamma),(b,\kappa)\}$ at time t if and only if

$$U_{G\square H}(t) \cdot D_a \otimes D_{\alpha\beta} \cdot U_{G\square H}(-t) = D_b \otimes D_{\gamma\kappa}.$$

By previous corollary, we have that

$$\begin{aligned} U_{G\Box H}(t) \cdot D_a \otimes D_{\alpha\beta} \cdot U_{G\Box H}(-t) &= U_{G\Box H}(t) \cdot D_a \otimes D_{\alpha\beta} \cdot (U_G(-t) \otimes U_H(-t)) \\ &= (U_G(t) \otimes U_H(t)) \cdot (D_a U_G(-t) \otimes D_{\alpha\beta} U_H(-t) \\ &= (U_G(t) D_a U_G(-t)) \otimes (U_H(t) D_{\alpha\beta} U_H(-t)) \\ &= D_b \otimes D_{\gamma\kappa}, \end{aligned}$$

which is equivalent to that there is perfect Laplacian state transfer between vertex a and b in G at time t and at the same time there is perfect state transfer between edge (α, β) and (γ, κ) in H . □

When we consider perfect edge state transfer in a Cartesian product of two graphs, we not only need to consider edge state transfer but also vertex state transfer with respect to the Laplacian matrix.

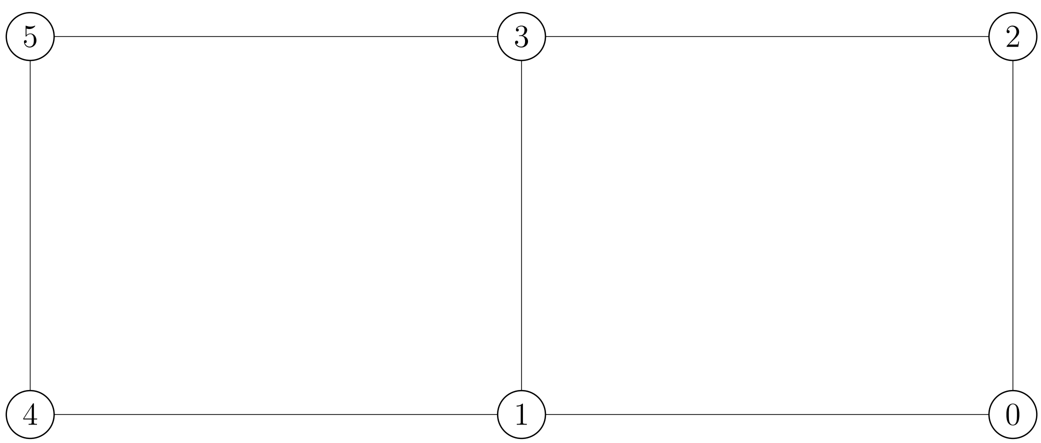

Figure 4.1: $P_2 \Box P_3$

The example given by Coutinho in [7, Section 2.4] shows that P_2 admits perfect state transfer with respect to its Laplacian matrix between its vertices at time $\frac{\pi}{2}$. Later on we will prove Theorem 5.4.7, which tells us that P_3 admits perfect edge state transfer between its edges at time $\frac{\pi}{2}$. By Theorem 4.2.3, there is perfect state transfer from $e_3 - e_5$ to $e_1 - e_0$ and from $e_2 - e_3$ to $e_1 - e_4$ in Figure 4.1.

4.3 Transitivity

Figure 4.2: the Complement of the Graph in Figure 4.1

The graph above is the complement of the graph in Figure 4.1. We know that there are perfect edges states transfer from $e_3 - e_5$ to $e_1 - e_0$ and from $e_2 - e_3$ to $e_1 - e_4$ in Figure 4.1.

By Theorem 4.1.2, we know that there are also perfect edge states transfer from $e_3 - e_5$ to $e_1 - e_0$ and from $e_2 - e_3$ to $e_1 - e_4$ in Figure 4.2. Actually the graph in Figure 4.2 also admits perfect edge state transfer between $e_2 - e_5$ and $e_0 - e_4$. This leads us to our next theorem about the transitivity phenomenon that occurs when there are two pairs of perfect edges state transfer in the same graph under certain conditions.

4.3.1 Theorem. *Suppose there is perfect state transfer between $e_a - e_b$ and $e_\alpha - e_\beta$ at time τ in G and there is also perfect state transfer between $e_b - e_c$ and $e_\beta - e_\gamma$ at the same time τ in G. Then there is perfect state transfer between $e_a - e_c$ and $e_\alpha - e_\gamma$ at time τ in G.*

Proof. Let D_{ab} denote the density matrix of $e_a - e_b$ and D_{bc} denote the density matrix of $e_b - e_c$. We have that

$$D_{ab} = \frac{1}{2}(e_a - e_b)(e_a - e_b)^T, \quad D_{bc} = \frac{1}{2}(e_b - e_c)(e_b - e_c)^T.$$

Using that

$$(e_a - e_b)^T(e_b - e_c) = (e_b - e_c)^T(e_a - e_b) = -1,$$

we can write the density matrix of $e_a - e_c$ in terms of D_{ab} and D_{bc} in the following way.

$$\begin{aligned}
D_{ac} &= \frac{1}{2}(e_a - e_c)(e_a - e_c)^T \\
&= \frac{1}{2}\left((e_a - e_b) + (e_b - e_c)\right)\left((e_a - e_b) + (e_b - e_c)\right)^T \\
&= \frac{1}{2}\big((e_a - e_b)(e_a - e_b)^T + (e_b - e_c)(e_b - e_c)^T \\
&+ (e_a - e_b)(e_b - e_c)^T + (e_b - e_c)(e_a - e_b)^T\big) \\
&= \frac{1}{2}\big((e_a - e_b)(e_a - e_b)^T + (e_b - e_c)(e_b - e_c)^T \\
&- (e_a - e_b)(e_a - e_b)^T(e_b - e_c)(e_b - e_c)^T \\
&- (e_b - e_c)(e_b - e_c)^T(e_a - e_b)(e_a - e_b)^T\big) \\
&= D_{ab} + D_{bc} - 2D_{ab}D_{bc} - 2D_{bc}D_{ab}
\end{aligned}$$

As the above shows, we have

$$D_{ac} = D_{ab} + D_{bc} - 2D_{ab}D_{bc} - 2D_{bc}D_{ab}.$$

Similarly, we have

$$D_{\alpha\gamma} = D_{\alpha\beta} + D_{\beta\gamma} - 2D_{\alpha\beta}D_{\beta\gamma} - 2D_{\beta\gamma}D_{\alpha\beta}.$$

Now consider $U(\tau)D_{ac}U(-\tau)$. Since we know that

$$U(\tau)D_{ab}U(-\tau) = D_{\alpha\beta} \quad \text{and} \quad U(\tau)D_{bc}U(-\tau) = D_{\beta\gamma},$$

we have

$$\begin{aligned}
U(\tau)D_{ac}U(-\tau) &= U(\tau)\left(D_{ab} + D_{bc} - 2D_{ab}D_{bc} - 2D_{bc}D_{ab}\right)U(-\tau) \\
&= D_{\alpha\beta} + D_{\beta\gamma} - 2U(\tau)D_{ab}D_{bc}U(-\tau) - 2U(\tau)D_{bc}D_{ab}U(-\tau).
\end{aligned}$$

Using $U(-\tau) \cdot U(\tau) = 1$, we get

$$U(\tau)D_{ab}D_{bc}U(-\tau) = U(\tau)D_{ab}U(-\tau) \cdot U(\tau)D_{bc}U(-\tau) = D_{\alpha\beta}D_{\beta\gamma}$$

and similarly,

$$U(\tau)D_{bc}D_{ab}U(-\tau) = U(\tau)D_{bc}U(-\tau) \cdot U(\tau)D_{ab}U(-\tau) = D_{\beta\gamma}D_{\alpha\beta}.$$

Thus, we get that

$$U(\tau)D_{ac}U(-\tau) = D_{\alpha\beta} + D_{\beta\gamma} - 2D_{\alpha\beta}D_{\beta\gamma} - 2D_{\beta\gamma}D_{\alpha\beta} = D_{\alpha\gamma}.$$

Therefore, there is perfect state transfer between $e_a - e_c$ and $e_\alpha - e_\gamma$ at time τ. □

By the monogamy property of perfect vertex state transfer, we know that for a vertex state e_a, it has at most one vertex state e_b such that there is perfect state transfer from e_a to e_b. By the symmetry of perfect state transfer, we know that there is perfect state transfer from e_b to e_a and again, by the monogamy property, there is no other state that e_b can be perfectly transferred to. Thus, the transitivity phenomenon can never happen in perfect vertex state transfer.

Chapter 5

Special Cases

In this chapter, we will characterize perfect edge state transfer in some special cases. One thing that distinguishes vertex states and edge states is that vertex states cannot have eigenvalue support of size one, but this is not rare for edge states. We will give characterizations of perfect state transfer and periodicity of edge states with eigenvalue support of size one. We also will show that there is always perfect edge state transfer in complete bipartite graph $K_{2,4n}$ for a positive integer n.

In addition, we show that C_4 is the only cycle and P_3, P_4 are the only paths that have perfect edge state transfer. In the last section, we make some comments on an interesting correspondence of perfect state transfer between graphs and their line graphs, which we observe during our investigation on perfect state transfer in paths and cycles.

5.1 Edge States with Eigenvalue Support of Size One

A vertex state in a connected graph with at least two vertices can never have eigenvalue support of size one, while an edge state with eigenvalue support of size one is not uncommon.

5.1.1 Lemma. *Let G be a graph and L denote the Laplacian of G with spectral decomposition $\sum_r \theta_r E_r$. Let (a,b) be an edge of G. For any non-zero eigenvalue θ_i that is not in the eigenvalue support of $e_a - e_b$, we must* *have that*

$$(E_i)_{aa} = (E_i)_{bb} = (E_i)_{ab} = (E_i)_{ba}.$$

Proof. Let θ_i be an eigenvalue that is not in the eigenvalue support of $e_a - e_b$. Then we know that

$$E_i(e_a - e_b) = 0$$
$$E_i e_a = E_i e_b,$$

which gives us

$$(E_i)_{aa} = (E_i)_{ab} \quad \text{and} \quad (E_i)_{bb} = (E_i)_{ba}.$$

Since the spectral idempotents of L are symmetric, we know that

$$(E_i)_{ab} = (E_i)_{ba}$$

for all i. Therefore,

$$(E_i)_{aa} = (E_i)_{bb} = (E_i)_{ab} = (E_i)_{ba}$$

for every θ_i that is not in the eigenvalue support of $e_a - e_b$. □

5.1.2 Lemma. *If (a, b) is an edge of G with eigenvalue support of size 1, then vertex a and vertex b have the same degree.*

Proof. Let (a, b) be an edge in graph G such that θ_j is the only eigenvalue in the eigenvalue support of $e_a - e_b$. Let L be the Laplacian matrix of G with spectral decomposition $\sum_r \theta_r E_r$. We know that $\sum_r E_r = I$, then we can have that

$$\sum_r (E_r)_{aa} = \sum_r (E_r)_{bb} = 1.$$

By Lemma 5.1.1, we know

$$(E_i)_{aa} = (E_i)_{bb}$$

for all $i \neq j$. Thus, we must have that

$$(E_j)_{aa} = (E_j)_{bb}.$$

Then we can have that

$$\deg(a) = L_{aa} = \sum_{r=0}^{r} \theta_r (E_r)_{aa} = \sum_{r=0}^{r} \theta_r (E_r)_{bb} = L_{bb} = \deg(b).$$

Thus, if $e_a - e_b$ has eigenvalue support of size 1, then vertex a and b have the same degree in G. □

5.1.3 Theorem. *Let (a, b) be an edge in graph G. If $e_a - e_b$ has eigenvalue support of size one, then $e_a - e_b$ is periodic for all time t, i.e.,*

$$\left| \frac{1}{2}(e_a - e_b)^T U(t)(e_a - e_b) \right|^2 = 1$$

for all t.

Proof. Let $U(t)$ denote the transition matrix associated with graph G and $\sum_r \theta_r E_r$ is the spectral decomposition of the Laplacian of G. Let θ_j be the only eigenvalue in the eigenvalue support of $e_a - e_b$. Then Lemma 5.1.1 allows us to have

$$\begin{aligned} \frac{1}{2}(e_a - e_b)^T U(t)(e_a - e_b) &= \frac{1}{2}\left(\sum_r e^{it\theta_r} \left((E_i)_{aa} + (E_i)_{bb} - 2(E_i)_{ab} \right) \right) \\ &= \frac{1}{2} e^{it\theta_j} \left((E_j)_{aa} + (E_j)_{bb} - 2(E_j)_{ab} \right) \\ &= \frac{1}{2} e^{it\theta_j} \cdot 2 \left((E_j)_{aa} - (E_j)_{ab} \right) \\ &= e^{it\theta_j} \left((E_j)_{aa} - (E_j)_{ab} \right) \end{aligned}$$

Since $\sum_r E_r = I$, we have $\sum_r (E_r)_{aa} = 1$ and $\sum_r (E_r)_{ab} = 0$. Since θ_j is the only eigenvalue in the eigenvalue support, Lemma 5.1.1 gives us that

$$\sum_r (E_r)_{aa} - \sum_r (E_r)_{ab} = (E_j)_{aa} - (E_j)_{ab} = 1.$$

It follows that

$$\frac{1}{2}(e_a - e_b)^T U(t)(e_a - e_b) = e^{it\theta_j}.$$

We know that

$$\left| e^{it\theta_j} \right|^2 = 1$$

for all t, which completes our proof. □

5.1.4 Theorem. *Let (a, b) be an edge in graph G such that the eigenvalue support of $e_a - e_b$ has size one. Then $e_a - e_b$ does not have perfect state transfer in G.*

Proof. Assume that (c, d) is an edge in G and there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ in G. Then by the Corollary 2.6.2, we know that $e_a - e_b$ and $e_c - e_d$ have the same eigenvalue support. So we assume that θ_j is the only eigenvalue in their eigenvalue support. Then we have that

$$\frac{1}{2}(e_c - e_d)^T U(t)(e_a - e_b) = \frac{1}{2}e^{it\theta_j}\left((E_j)_{ac} + (E_j)_{ad} - (E_j)_{bc} + (E_j)_{bd}\right).$$

Since $\sum_r E_r = I$, we can have that if (a, b) and (c, d) has one common vertex,

$$\sum_r \left((E_r)_{ac} + (E_r)_{bd} - (E_r)_{ad} + (E_r)_{bd}\right) = 1,$$

and if they have no common vertex,

$$\sum_r \left((E_r)_{ac} + (E_r)_{bd} - (E_r)_{ad} + (E_r)_{bd}\right) = 0.$$

Since θ_r is the only element in the eigenvalue support, we have that

$$(E_j)_{ac} + (E_j)_{ad} - (E_j)_{bc} + (E_j)_{bd} = 0$$

for all $j \neq r$. Thus, we get that

$$\begin{aligned}&\sum_r \left((E_r)_{ac} + (E_r)_{bd} - (E_r)_{ad} + (E_r)_{bd}\right)\\ &= (E_r)_{ac} + (E_r)_{bd} - (E_r)_{ad} + (E_r)_{bd}\\ &= 0 \text{ or } 1\end{aligned}$$

Hence, we have that

$$\left|\frac{1}{2}(e_c - e_d)^T U(t)(e_a - e_b)\right|^2 = \left|\frac{1}{2}e^{it\theta_r}\left((E_r)_{ac} + (E_r)_{ad} - (E_r)_{bc} + (E_r)_{bd}\right)\right|,$$

which is

$$\left|\frac{1}{2}e^{it\theta_r}\right|^2 = \frac{1}{4}$$

if (a, b) and (c, d) have one common vertex or 0 if they have no common vertex. But there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$ if and only if

$$\left|\frac{1}{2}(e_c - e_d)^T U(t)(e_a - e_b)\right|^2 = 1.$$

We can conclude that there is no such state $e_c - e_d$ in G that there is perfect state transfer between $e_a - e_b$ and $e_c - e_d$. Therefore, there is no perfect state transfer starting at $e_a - e_b$ in G. □

Since zero is always an eigenvalue of the Laplacian of a graph with the corresponding eigenvector being the all-one vector, we know that zero cannot be in the eigenvalue support of any edges of any graphs. For complete graphs, we know that the eigenvalue support of any edge is always of size one, which allows us to derive the following corollary.

5.1.5 Corollary. *Every edge in a complete graph is periodic but has no perfect state transfer.* □

5.2 Complete Bipartite $K_{2,4n}$

The *complete bipartite graph* $K_{m,n}$ consists of an independent set of m vertices completely joined to an independent set of n vertices. Throughout this section, we use $K_{2,4n}$ to denote a complete bipartite graph for some positive integer n. Let A and B be two parts of $K_{2,4n}$ such that $V(A) = \{v_1, v_2\}$ and $V(B) = \{v_3, v_4, \cdots, v_{4n+2}\}$. Also, we use I_n to denote the identity matrix of order $n \times n$ and J_n to denote the all-one matrix of order $n \times n$.

In this section, we show that there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ in $K_{2,4n}$ for $i \in \{3, 4, \cdots, 4n+2\}$ at time $\frac{\pi}{2}$.

5.2.1 Lemma. *Let superscripts denote the multiplicities of the eigenvalues. Then the Laplacian eigenvalues of* $K_{2,4n}$ *are* $0^{(1)}, 2^{(4n-1)}, 4n^{(1)}, 4n+2^{(1)}$.

Proof. Since $K_{2,4n}$ has only one connected component, zero is always an Laplacian eigenvalue with multiplicity one.
Let H be the complement of $K_{2,4n}$, which is a disjoint union of complete graphs K_2 and K_{4n} and we have

$$V(K_2) = \{v_1, v_2\}, \quad V(K_{4n}) = \{v_3, v_4, \cdots, v_{4n+2}\}.$$

Since K_2 has eigenvalues $\{0^{(1)}, 2^{(1)}\}$ and K_{4n} has eigenvalues $\{0^{(1)}, 4n^{(4n-1)}\}$, by Lemma 4.1.1, H has eigenvalues $\{2^{(4n-1)}, 4n^{(1)}\}$. By computations, one can easily verify that $4n+2$ is always a Laplacian eigenvalue with the spectral idempotent

$$E(4n+2) = \frac{1}{2+1/n}\left(\begin{array}{cc|cccc} 1 & 1 & -\frac{1}{2n} & -\frac{1}{2n} & \cdots & -\frac{1}{2n} \\ 1 & 1 & -\frac{1}{2n} & -\frac{1}{2n} & \cdots & -\frac{1}{2n} \\ \hline -\frac{1}{2n} & -\frac{1}{2n} & & & & \\ -\frac{1}{2n} & -\frac{1}{2n} & & & & \\ \vdots & \vdots & & \frac{1}{4n^2}J_{4n} & & \\ \vdots & \vdots & & & & \\ -\frac{1}{2n} & -\frac{1}{2n} & & & & \end{array}\right).$$

□

It is not hard to verify that the spectral idempotent of eigenvalue 2 is

$$E(2) = \frac{1}{4n}\left(\begin{array}{cc|cccc} 0 & 0 & 0 & 0 & \cdots & 0 \\ 0 & 0 & 0 & 0 & \cdots & 0 \\ \hline 0 & 0 & & & & \\ 0 & 0 & & & & \\ \vdots & \vdots & & 4nI_{4n} - J_{4n} & & \\ \vdots & \vdots & & & & \\ 0 & 0 & & & & \\ 0 & 0 & & & & \end{array}\right).$$

Similarly, we can also verify that the spectral idempotent of eigenvalue $4n$ is

$$E(4n) = \frac{1}{2}\begin{pmatrix} 1 & -1 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & 0 \\ 0 & 0 & 0 & \cdots & 0 \end{pmatrix},$$

which has 0 everywhere except for the upper left 2×2-block.

Since 0 is never in the eigenvalue support of an edge state, spectral idempotents of non-zero eigenvalues are enough to help us to derive the theorem below.

5.2.2 Theorem. *There is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ in $K_{2,4n}$ for $i \in \{3, 4, \cdots, 4n+2\}$ at time $\frac{\pi}{2}$.*

Proof. Let

$$a_j = (E(j))_{12} + (E(j))_{1i} - (E(j))_{2i} + (E(j))_{ii}$$

for all non-zero eigenvalue j. We have that

$$\begin{aligned}
\left|\frac{1}{2}(e_1 - e_i)^T U(t)(e_2 - e_i)\right|^2 &= \left|\frac{1}{2}\sum_r e^{it\theta_r}\left(E(r)_{12} - E(r)_{1i} - E(r)_{2i} + E(r)_{ii}\right)\right|^2 \\
&= \frac{1}{4}\left(\sum_r a_r^2 + \sum_{r\neq s} 2a_r a_s \cos(\theta_s t - \theta_r t)\right) \\
&= \frac{1}{4}\big(a_2^2 + a_{4n}^2 + a_{4n+2}^2 + 2a_2 a_{4n}\cos(4n-2)t \\
&+ 2a_2 a_{4n+2}\cos 4nt + 2a_{4n}a_{4n+2}\cos 2t\big).
\end{aligned}$$

From the idempotents shown before, we have that

$$\begin{aligned}
a_{4n} &= E(4n)_{12} - E(4n)_{1i} - E(4n)_{2i} + E(4n)_{ii} = -\frac{1}{2}, \\
a_2 &= E(2)_{12} - E(2)_{1i} - E(2)_{2i} + E(2)_{ii} \\
&= \frac{1}{4n}(0 - 0 - 0 + 4n - 1) \\
&= 1 - \frac{1}{4n}, \\
a_{4n+2} &= E(4n+2)_{12} - E(4n+2)_{1i} - E(4n+2)_{2i} + E(4n+2)_{ii} \\
&= \frac{1}{2+\frac{1}{n}}\left(1 + \frac{1}{2n} + \frac{1}{2n} + \frac{1}{4n^2}\right) \\
&= \frac{2n+1}{4n}.
\end{aligned}$$

When $t = \frac{\pi}{2}$, we have that

$$\begin{aligned}\left|\frac{1}{2}(e_1 - e_i)^T U(t)(e_2 - e_i)\right|^2 &= \frac{1}{4}\big(a_2^2 + a_{4n}^2 + a_{4n+2}^2 + 2a_2a_{4n}\cos(2n-1)\pi \\ &+ 2a_2a_{4n+2}\cos 2n\pi + 2a_{4n}a_{4n+2}\cos\pi\big) \\ &= \frac{1}{4}\left(a_2^2 + a_{4n}^2 + a_{4n+2}^2 - 2a_2a_{4n} + 2a_2a_{4n+2} - 2a_{4n}a_{4n+2}\right) \\ &= \frac{1}{4}\left(a_{4n}(a_{4n} - 2a_2 - 2a_{4n+2}) + (a_2 + a_{4n+2})^2\right) \\ &= \frac{1}{4}\left(-\frac{1}{2}\cdot\left(-\frac{1}{2} - 3\right) + \left(\frac{3}{2}\right)^2\right) \\ &= 1.\end{aligned}$$

This implies that there is perfect state transfer between $e_1 - e_i$ and $e_2 - e_i$ at time $\frac{\pi}{2}$ in $K_{2,4n}$. □

The author does not know yet perfect edge state transfer in complete bipartite graphs of any other forms except for $K_{2,4n}$ where n is a positive integer.

5.3 Cycles

Throughout this section, we use C_n to denote the cycle on n vertices and $A(C_n), L(C_n)$ to denote the adjacency and Laplacian matrix of C_n respectively.

In this section, we use a bound on n such that C_n can have a periodic edge state to eliminate the cases when C_n can have perfect state transfer. We show that C_4 is the only cycle that has perfect state transfer.

5.3.1 Lemma. *The eigenvectors of adjacency matrix of C_n are*

$$v_k = \begin{pmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(n-1)k} \end{pmatrix}$$

for $k = 0, 1, \cdots, n-1$ *and* $\omega = e^{\frac{2\pi}{n}i}$ *with the corresponding eigenvalues*

$$2\cos\left(\frac{2\pi k}{n}\right).$$

Proof. Let W be a $n \times n$ matrix with

$$\begin{aligned} &W_{i,i+1} = 1, \quad i = 1, 2, \cdots, n-1, \\ &W_{n,1} = 1 \end{aligned}$$

and zero everywhere else. We can see that W is just a permutation matrix and hence, it is not hard to see that W^{-1} is a $n \times n$ matrix with

$$\begin{aligned} &W_{i,i-1} = 1, \quad i = 2, \cdots, n, \\ &W_{1,n} = 1 \end{aligned}$$

and zero everywhere else. The adjacency matrix of C_n is

$$A(C_n) = W + W^{-1}.$$

Let

$$v = \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix}$$

denote an eigenvector of W with eigenvalue λ. Since W acts on each vector by shifting each entry up by one position with the first entry becoming the last, we have that

$$Wv = W \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = \begin{pmatrix} v_2 \\ v_3 \\ \vdots \\ v_1 \end{pmatrix} = \lambda \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix},$$

which gives us that

$$v_1 = \lambda v_n = \lambda^2 v_{n-1} = \lambda^3 v_{n-2} = \cdots = \lambda^n v_1.$$

Thus, we have that

$$\lambda^n = 1.$$

Notice that there is no v_i such that $v_i = 0$, otherwise the equation above will make all the entries of v zero. We know that the eigenvalues of W are among the n-th roots of unity and all the eigenvalues of C_n are real, so all the eigenvalues are in the form of ω^k for some $k = 0, 1, \cdots, n-1$ with

$$\omega = e^{\frac{2\pi}{n} i}.$$

Now if we let $v_1 = 1$, we can see that the eigenvector with eigenvalue ω^k is

$$v_k = \begin{pmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(n-1)k} \end{pmatrix}$$

for $k = 0, 1, \cdots, n-1$ and hence, for each $k \in \{0, 1, 2, \cdots, n-1\}$, ω^k is an eigenvalue with multiplicity 1. It follows that W^{-1} has eigenvectors v_k with eigenvalues $1/w^k$ for $k = 0, 1, \cdots, n-1$. Thus, we have that

$$A(C_n)v_k = \left(\omega^k + \frac{1}{\omega^k}\right) v_k.$$

Therefore, the eigenvectors of $A(C_n)$ are

$$\begin{pmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(n-1)k} \end{pmatrix}$$

for $k = 0, 1, \cdots, n-1$ with eigenvalues

$$\omega^k + \omega^{-k} = e^{\frac{2\pi k}{n} i} + e^{-\frac{2\pi k}{n} i} = 2\cos\left(\frac{2\pi k}{n}\right).$$

$\square$

Using the fact that C_n is a regular graph, we can easily derive the Laplacian eigenvalues and eigenvectors from the eigenvalues and the eigenvectors of $A(C_n)$.

5.3.2 Lemma. *Laplacian eigenvectors of C_n are*

$$v_k = \begin{pmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(n-1)k} \end{pmatrix}$$

for $k = 0, 1, \cdots, n-1$ where $\omega = e^{\frac{2\pi}{n}i}$ with eigenvalues

$$2 - 2\cos\frac{2\pi k}{n}$$

for $k = 0, 1, \cdots, n-1$.

Proof. Since C_n is a regular graph with valency 2, we know that the Laplacian of C_n is

$$L = 2I - A(C_n).$$

Let v_k be the eigenvector of $A(C_n)$ as defined in Lemma 5.3.1 with eigenvalue

$$2\cos\frac{2\pi k}{n}$$

for $k = 0, 1, \cdots, n-1$, we have that

$$Lv_k = (2I - A(C_n))\, v_k = \left(2 - 2\cos\frac{2\pi k}{n}\right) v_k.$$

Therefore, Laplacian eigenvalues of C_n are

$$2 - 2\cos\frac{2\pi k}{n}$$

with corresponding eigenvectors v_k for $k = 0, 1, \cdots, n-1$. □

5.3.3 Lemma. *every edge state of C_n has eigenvalue support of size $\lfloor \frac{n}{2} \rfloor$.*

Proof. From Lemma 5.3.1, We know that a Laplacian eigenvector of C_n is

$$v_k = \begin{pmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(n-1)k} \end{pmatrix}$$

for some $k \in \{0, 1, \cdots, n-1\}$ and $\omega = e^{\frac{2\pi}{n}i}$ and the corresponding eigenvalue is $\theta_k = 2 - 2\cos(2\pi k/n)$. Let u_k be a vector of length n such that

$$u_k = \omega^k v_k = \begin{pmatrix} \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{nk} \end{pmatrix}$$

for some $k \in \{0, 1, \cdots, n-1\}$. We can see that the j-th entry of u_k is

$$(u_k)_j = \omega^{jk}, \quad j = 1, 2, \cdots, n.$$

Then u_k is also an eigenvector of $L(C_n)$ with the same eigenvalue as v_k, i.e.,

$$L(C_n)u_k = \left(2 - 2\cos\frac{2\pi k}{n}\right) u_k.$$

We can write

$$(u_k)_j = \omega^{jk} = \left(e^{\frac{2\pi}{n}i}\right)^{jk} = \sin\left(\frac{2jk\pi}{n}\right) + i\cos\left(\frac{2jk\pi}{n}\right)$$

and we can see that u_k is a complex vector. Let $u_k = a_k + b_k i$ where a_k, b_k are real vectors of length n such that

$$(a_k)_j = \sin\left(\frac{2jk\pi}{n}\right), \quad (b_k)_j = \cos\left(\frac{2jk\pi}{n}\right), \quad j = 1, 2, \cdots, n.$$

Then we have

$$L(C_n)u_k = L(C_n)\left(a_k + ib_k\right) = \left(2 - 2\cos\frac{2\pi k}{n}\right)\left(a_k + ib_k\right).$$

Since $L(C_n)$ is a real matrix and all the eigenvalues of $L(C_n)$ are real, we must have that

$$L(C_n)a_k = \left(2 - 2\cos\frac{2\pi k}{n}\right)a_k, \quad L(C_n)b_k = \left(2 - 2\cos\frac{2\pi k}{n}\right)b_k.$$

We can see that a_k, b_k are both real eigenvectors with the same eigenvalue $2 - 2\cos(2\pi k/n)$.
Since we have

$$\cos\frac{2\pi(n-r)}{n} = \cos\left(2\pi - \frac{2\pi r}{n}\right) = \cos\frac{2\pi r}{n},$$

we know that $k = r$ and $k = n - r$ produce the same eigenvalue for $r \in \{1, 2, \cdots, n-1\}$. Thus, we can conclude that $L(C_n)$ has $\lceil\frac{n-1}{2}\rceil$ distinct non-zero eigenvalues. When n is odd, all the non-zero eigenvalues of $L(C_n)$ have multiplicity two. When n is even and $k = n/2$, we have that $b_k = \mathbf{0}$ and hence, the multiplicity of θ_k is one for $k = n/2$ and all the non-zero θ_k have multiplicity two for $k \neq n/2$.

Now consider the eigenvalue support of $e_{n-1} - e_n$,

$$(a_k)_n = \sin\left(\frac{2kn\pi}{n}\right) = 0$$

for all $k \in \{1, 2, \cdots, n-1\}$ while since $k < n$ and $n \geq 3$, we know that

$$(a_k)_n = \sin\left(\frac{2k(n-1)\pi}{n}\right) \neq 0$$

for all $k \in \{1, 2, \cdots, n-1\}$. Thus, all the non-zero eigenvalues of $L(C_n)$ are in the eigenvalue support of $e_{n-1} - e_n$, which means that it has eigenvalue support of size $\lceil\frac{n-1}{2}\rceil = \lfloor\frac{n}{2}\rfloor$.
Since C_n is edge-transitive, by Corollary 2.6.4, we know that all the edge states of C_n have the same eigenvalue support. we can conclude that the size of the eigenvalue support of an edge in C_n is $\lfloor\frac{n}{2}\rfloor$. □

Corollary 3.2.8 and the previous lemma help us to derive an upper bound on n such that C_n can have a periodic edge state. Since periodicity is a necessary condition for an edge state to have perfect state transfer, we can eliminate the number of n such that C_n can have perfect edge state transfer.

5.3.4 Theorem. *There is perfect edge state transfer in C_n if and only if $n = 4$.*

Proof. By Lemma 5.3.2, we know that the Laplacian eigenvalues of C_n are

$$0 \leq 2 - 2\cos\left(\frac{2\pi k}{n}\right) \leq 4$$

for $k = 0, 1, \cdots, n-1$. By Corollary 3.2.8, we know that for an edge state to be periodic, the size of eigenvalue support must be at most 4. Then by Lemma 5.3.3, we know that for C_n to have a periodic edge state, we must have $3 \leq n \leq 9$.

Using Theorem 3.2.7, we can find that there are no periodic edge states in C_n when $n = 7, 8, 9$ which implies that there is no perfect edge state transfer in C_n. Since cycles are edge-transitive, by Corollary 3.4.8, we know there is no perfect state transfer in C_3 and C_5. Computing

$$\left|\frac{1}{2}(e_a - e_b)^T U(t)(e_c - e_d)\right|^2$$

for all distinct edges $(a, b), (c, d)$ in $E(C_n)$ when $n = 4, 6$, we can conclude that the only cycle that has perfect edge state transfer is C_4. □

At time $\frac{\pi}{2}$, there is perfect state transfer between the opposite edges in C_4.

5.4 Paths

In this section, we let P_n denote the path on n vertices such that $V(P_n) = \{1, 2, \cdots, n\}$. We use $A(P_n)$ to denote the adjacency matrix of P_n and $L(P_n)$ to denote the Laplacian matrix of P_n. We show that P_3, P_4 are the only two paths where perfect edge state transfer can occur.

The original proof of the following lemmas and theorems about the Laplacian eigenvalues and the Laplacian eigenvectors can be found in [8, Section 12.2,12.5].

5.4.1 Lemma. *Laplacian eigenvalues of P_n are*

$$2 - 2\cos\frac{\pi r}{n}$$

for $r = 0, 1, \cdots, n-1$.

Proof. Let Δ denote the degree matrix of P_n and L denote the Laplacian matrix of P_n. We have that $L = \Delta - A(P_n)$.
Let B be the $n \times (n-1)$ matrix with

$$B_{i,i} = 1, \quad B_{i,i-1} = -1$$

and all the other entries zero. Then we have that

$$BB^T = \Delta - A(P_n) \quad \text{and} \quad B^T B = 2I - A(P_{n-1}).$$

Let $E_1, E_2, \cdots, E_{n-1}$ be the idempotents in the spectral decomposition of $A(P_{n-1})$. Then we have that

$$\begin{aligned} (\Delta - A(P_n))\, BE_r B^T &= BB^T BE_r B^T \\ &= B\,(2I - A(P_{n-1}))\, E_r B^T \\ &= B(2-\theta_r)E_r B^T \\ &= (2-\theta_r)BE_r B^T, \end{aligned}$$

where θ_r is the eigenvalue of $A(P_{n-1})$ with E_r being its corresponding spectral idempotent. Since the eigenvalues of $A(P_{n-1})$ are

$$2\cos\frac{\pi r}{n}$$

for $r = 0, 1, \cdots, n-1$, we can see that $BE_r B^T$'s and J are all the spectral idempotents of $\Delta - A(P_n)$ with eigenvalue

$$2 - \theta_r = 2 - 2\cos\frac{\pi r}{n}$$

for $r = 0, 1, \cdots, n-1$. □

Since $r = 0, 1, \cdots, n-1$ and $\frac{r}{n} < 1$, we know that all the Laplacian eigenvalues of P_n are simple. From the proof of Lemma 5.4.1, we can see that the spectral idempotents of $A(P_{n-1})$ help us to obtain the Laplacian eigenvectors of P_n.

5.4.2 Lemma.

$$2\sum_{r=0}^{n}\cos(r\theta) = \frac{\sin\left((n+\frac{1}{2})\theta\right)}{\sin\left(\frac{1}{2}\theta\right)} + 1$$

Proof. Let $q = e^{i\theta} = \cos\theta + i\sin\theta$. We have that

$$\begin{aligned}
2\sum_{r=0}^{n}\cos(r\theta) = \sum_{r=0}^{n}\left(e^{ir\theta}+e^{-ir\theta}\right) &= \sum_{r=0}^{n}\left(q^r+q^{-r}\right) \\
&= \frac{q^{n+1}-1}{q-1} + \frac{q^{-n-1}-1}{q^{-1}-1} \\
&= \frac{q^{n+1/2}-q^{-1/2-n}}{q^{1/2}-q^{-1/2}} + 1 \\
&= \frac{\sin\left((n+\frac{1}{2})\theta\right)}{\sin\left(\frac{1}{2}n\right)} + 1,
\end{aligned}$$

which completes our proof. □

5.4.3 Lemma. *The idempotents $E_1, E_2, \cdots, E_n$ in the spectral decomposition of $A(P_n)$ are given by*

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

for $1 \le j,k \le n$.

Proof. Let e_n denote the n-th vector in the standard basis of $\mathbb{R}^n$. Using the trigonometric identity

$$2\sin x\cos y = \sin(x+y) + \sin(x-y),$$

we have that

$$A(P_n)\begin{pmatrix}\sin(\beta)\\ \sin(2\beta)\\ \sin(3\beta)\\ \vdots\\ \sin(n\beta)\end{pmatrix} = \begin{pmatrix}\sin(2\beta)\\ \sin(\beta)+\sin(3\beta)\\ \sin(2\beta)+\sin(4\beta)\\ \vdots\\ \sin((n-2)\beta)+\sin(n\beta)\\ \sin((n-1)\beta)\end{pmatrix}$$

$$= 2\cos(\beta)\begin{pmatrix}\sin(\beta)\\ \sin(2\beta)\\ \sin(3\beta)\\ \vdots\\ \sin((n-1)\beta)\\ \sin(n\beta)\end{pmatrix} - \sin\left((n+1)\beta\right)e_n$$

If $\sin\left((n+1)\beta\right)=0$, then

$$z(\beta) := \begin{pmatrix}\sin(\beta)\\ \sin(2\beta)\\ \sin(3\beta)\\ \vdots\\ \sin((n-1)\beta)\\ \sin(n\beta)\end{pmatrix}$$

is an eigenvector of $A(P_n)$ with eigenvalue $2\cos\beta$. Let β vary over the values

$$\frac{\pi r}{n+1}$$

for $r = 1, 2, \cdots, n$ and then we get n distinct eigenvalues. Thus, each eigenvalue of $A(P_n)$ is simple and the corresponding spectral idempotent is

$$\frac{1}{z(\beta)^T z(\beta)} z(\beta)z(\beta)^T.$$

Using Lemma 5.4.2, we have that

$$\begin{aligned}\sum_{k=0}^{n} \sin^2(k\beta) &= \sum_{r=0}^{n} \frac{1}{2}\left(1-\cos(2k\beta)\right)\\ &= \frac{n+1}{2} - \frac{1}{4}\left(\frac{\sin\left((2n+1)\beta\right)}{\sin(\beta)}+1\right).\end{aligned}$$

Since $\beta = \frac{\pi r}{n+1}$, we have that $(2n+1)\beta = 2r\pi - \beta$. We know that r is an integer, so that

$$\frac{\sin\left((2n+1)\beta\right)}{\sin(\beta)} = \frac{\sin\left(4r\pi - \beta\right)}{\sin\beta} = \frac{-\sin\beta}{\sin\beta} = -1.$$

Thus, we have that

$$\sum_{k=0}^{n} \sin^2\left(k\beta\right) = \frac{n+1}{2},$$

which gives us that

$$z(\beta)^T z(\beta) = \sum_{k=1}^{n} \sin^2(k\beta) = \sum_{k=0}^{n} \sin^2(j\beta) = \frac{n+1}{2}.$$

Therefore, we get that

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

□

5.4.4 Lemma. *The Laplacian eigenvector with eigenvalue* $2 - 2\cos\frac{\pi r}{n}$ *of* P_n *is*

$$2\sin\left(\frac{r\pi}{2n}\right)\begin{pmatrix} \cos\left(1\frac{r\pi}{2n}\right) \\ \cos\left(3\frac{r\pi}{2n}\right) \\ \cos\left(5\frac{r\pi}{2n}\right) \\ \vdots \\ \cos\left((2n-3)\frac{r\pi}{2n}\right) \\ \cos\left((2n-1)\frac{r\pi}{2n}\right) \end{pmatrix}$$

for $r = 0, 1, \cdots, n-1$.

Proof. Let $\sum_r \theta_r E_r$ denote the spectral decomposition of $A(P_{n-1})$ and L denote the Laplacian matrix of P_n. From Lemma 5.4.3, we know that

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

Let $\alpha = \frac{r\pi}{n}$ and let σ denote the column vector of length $n-1$ where $\sigma_j = \sin(j\alpha)$. Also, we let B be the matrix defined as in Lemma 5.4.1. Then

$$BE_rB^T = \frac{2}{n} B\sigma(B\sigma)^T.$$

In the proof of Lemma 5.4.1, we have already shown that

$$L\left(BE_rB^T\right) = (2-\theta_r)\left(BE_rB^T\right)$$

and hence, we know that $B\sigma$ is an eigenvector of L with eigenvalue $2-\theta_r$. By our definition of B and σ, we have

$$B\sigma = \begin{pmatrix} \sin(\alpha) \\ \sin(2\alpha)-\sin(\alpha) \\ \sin(3\alpha)-\sin(2\alpha) \\ \vdots \\ \sin((n-1)\alpha)-\sin((n-2)\alpha) \\ -\sin((n-1)\alpha) \end{pmatrix}.$$

Using the trigonometric identity

$$\sin(u)-\sin(v) = 2\cos\left(\frac{u+v}{2}\right)\sin\left(\frac{u-v}{2}\right),$$

we get that

$$B\sigma = 2\sin\left(\frac{\alpha}{2}\right)\begin{pmatrix} \cos\left(1\frac{\alpha}{2}\right) \\ \cos\left(3\frac{\alpha}{2}\right) \\ \cos\left(5\frac{\alpha}{2}\right) \\ \vdots \\ \cos\left((2n-3)\frac{\alpha}{2}\right) \\ \cos\left((2n-1)\frac{\alpha}{2}\right) \end{pmatrix},$$

where we use the fact that $n\alpha = r\pi$ to compute the last entry, whence $\sin(n\alpha)=0$ and we have

$$-\sin\left((n-1)\alpha\right) = \sin(n\alpha)-\sin\left((n-1)\alpha\right).$$

□

Now we want to use the Laplacian eigenvectors of P_n to give a bound on the size of eigenvalue support of an edge state in P_n. First, we prove that the sizes of the eigenvalue supports of edge states in P_n is symmetric. We can also prove the following lemma using automorphisms of path graphs and Theorem 2.6.3.

5.4.5 Lemma. *Let $(k, k+1)$ be an edge of P_n with $1 \leq k \leq n-1$. Then the eigenvalue supports of the edge states associated with $(k, k+1)$ and $(n-k, n-k+1)$ are the same.*

Proof. Let E_r denote the spectral idempotent of $L(P_n)$ with eigenvalue $2 - 2\cos(\pi r/n)$. Let v_r denote the eigenvector of $L(P_n)$ such that

$$v_r v_r^T = E_r.$$

Assume that $2 - 2\cos(\pi r/n)$ is not in the eigenvalue support of $(k, k+1)$, which means that

$$E_r (e_k - e_{k+1}) = 0.$$

Then we know that

$$v_r e_k^T = v_r e_{k+1}^T.$$

By Lemma 5.4.4, we must have that

$$\cos((2k-1)\frac{r\pi}{2n}) = \cos\left((2k+1)\frac{r\pi}{2n}\right).$$

Using the trigonometric identity

$$\cos(x) - \cos(y) = -2\sin\left(\frac{x+y}{2}\right)\sin\left(\frac{x-y}{2}\right),$$

we can have that

$$\cos((2k-1)\frac{r\pi}{2n}) - \cos\left((2k+1)\frac{r\pi}{2n}\right) = -2\sin\left(4k\frac{r\pi}{4n}\right)\sin\left(\frac{r\pi}{2n}\right) = 0. \tag{5.4.1}$$

Thus, if the integer r such that $1 \leq r \leq n-1$ and satisfies the equation above, then $2 - 2\cos(\pi r/n)$ is a non-zero eigenvalue not in the eigenvalue support of the edge state $(k, k+1)$.
Similarly, we know that the integer r such that $1 \leq r \leq n-1$ and satisfies

$$\cos\left((2(n-k)-1)\frac{r\pi}{2n}\right) = \cos\left((2(n-k)+1)\frac{r\pi}{2n}\right), \tag{5.4.2}$$

then $2 - 2\cos(\pi r/n)$ is a non-zero eigenvalue not in the eigenvalue support of $(n-k, n-k+1)$. Using the same trigonometric identity as above, we get

$$\begin{aligned}
&\cos\left((2(n-k)-1)\frac{r\pi}{2n}\right) - \cos\left((2(n-k)+1)\frac{r\pi}{2n}\right)\\
&= -2\sin\left(4(n-k)\frac{r\pi}{4n}\right)\sin\left(\frac{r\pi}{2n}\right)\\
&= -2\sin\left(r\pi - 4k\frac{r\pi}{4n}\right)\sin\left(\frac{r\pi}{2n}\right)\\
&= -2\left((-1)^r\sin(4k\frac{r\pi}{2n})\right)\sin\left(\frac{r\pi}{2n}\right)\\
&= 0.
\end{aligned}$$

Thus, we know that r satisfies Equation 5.4.1 if and only if r satisfies Equation 5.4.2. Therefore, the edge states associated with $(k, k+1)$ and $(n-k, n-k+1)$ have the same eigenvalue support. □

The symmetry of the eigenvalue supports of the edge state of P_n can help us to give a bound on the size of the eigenvalue support of an edge state in P_n.

5.4.6 Lemma. *Let S denote the eigenvalue support of an edge state in P_n. Then*

$$|S| \geq \frac{n}{2}.$$

Proof. We want to prove that there are at most $n/2$ eigenvalues that are not in the eigenvalue support of an edge state in P_n. Since 0 is never in the eigenvalue support of any edge state, we may assume that $2 - 2\cos(\pi r/n)$ is a non-zero eigenvalue that is not in the eigenvalue support of $e_k - e_{k+1}$ for some integer $1 \leq r \leq n-1$. The proof of Lemma 5.4.5 tells us that r must satisfy

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

Thus, we know that either

$$\frac{kr}{n} \quad \text{or} \quad \frac{r}{2n}$$

is an integer. But $1 \leq r \leq n-1$ and so

$$\frac{kr}{n} = z$$

for some positive integer z. Since $1 \le r \le n-1$, we know that z must satisfy that

$$1 \le \frac{n}{k} z \le n-1.$$

The number of z satisfying the inequality above is the number of non-zero eigenvalues not in the eigenvalue support of $e_k - e_{k+1}$. By Lemma 5.4.5, we only need to consider the cases when $k = 1, 2, \cdots, \lfloor \frac{n}{2} \rfloor$. Since the number of valid z decreases as the value of k increases and when $k = \lfloor \frac{n}{2} \rfloor$, the values that z can take is at most

$$\lfloor \frac{n}{2} \rfloor - 1 \le \frac{n}{2} - 1.$$

As stated before, zero is never in the eigenvalue support of an edge state and so, we can conclude that there are at most $n/2$ eigenvalues that are not in the eigenvalue support of an edge state in P_n. Therefore, the size of the eigenvalue support of an edge state is at least $n/2$. □

Periodicity is required for a state to have perfect state transfer. Corollary 3.2.8 states that if an edge state is periodic, then any two distinct eigenvalues in the eigenvalue support must differ by at least one. Since the Laplacian eigenvalues of P_n is bounded, we can have a bound on the number of vertices of a path graph that has periodic edge states.

5.4.7 Theorem. *A path graph on n vertices has perfect edge state transfer if and only if $n = 3, 4$.*

Proof. By Lemma 5.4.1, we know that P_n has Laplacian eigenvalue

$$0 \le 2 - 2\cos\frac{\pi r}{n} \le 4$$

for $r = 0, 1, \cdots, n-1$. By Corollary 3.2.8, we know that if an edge state of P_n is periodic, then its eigenvalue support has size at most four. Lemma 5.4.6 tells us that the eigenvalue support of an edge state of P_n is at least $n/2$. Thus, we know that for $n \ge 9$, there is no periodic edge states in P_n, which implies that there is no perfect state transfer in P_n when $n \ge 9$. Thus, we only need to consider the cases when $n = 3, 4, 5, 6, 7, 8$.

Using Theorem 3.2.7 we find that when $n = 5, 7, 8, 9$, there is no periodic edge states in P_n and also that, there is only one periodic edge state in P_6. If the vertices of P_6 from one end to the other are $0, 1, \cdots, 5$, then $e_2 - e_3$ is the only periodic state with period $2\sqrt{3}\pi/3$. Since if an edge state has perfect state transfer, then it must be periodic, which tells us that when $n = 5, 6, 7, 8, 9$, there is no perfect edge state transfer in P_n.

By computing

$$\left|\frac{1}{2}(e_a - e_b)^T U(t)(e_c - e_d)\right|^2$$

for all distinct edges $(a, b), (c, d)$ in $E(P_3)$ and $E(P_4)$, we find that there is perfect state transfer in P_3 and P_4. Therefore, there is perfect state transfer in P_n if and only if $n = 3, 4$. □

When $n = 3$, there is perfect state transfer between its edges in P_3 at time $\pi/2$. When $n = 4$, perfect state transfer occurs between two edges on its ends in P_4 at time $\sqrt{2}\pi/2$.

5.5 Comments

Stevanović [17] and Godsil [12] prove that P_n admits perfect vertex state transfer relative to adjacency matrices if and only if $n = 2$ or 3. Perfect vertex state transfer in P_2 happens between its two vertices at time $\pi/2$ and perfect vertex state transfer in P_3 happens between its end-vertices at time $\sqrt{2}\pi/2$.

In Section 5.4, we proved that P_n admits perfect edge state transfer only when $n = 3$ or 4 and

(i) there is perfect state transfer between its edges in P_3 at time $\pi/2$,

(ii) when $n = 4$, perfect state transfer occurs between two edges on its ends in P_4 at time $\sqrt{2}\pi/2$.

Later in Section 6.2, we will prove an analogous result for quantum walks relative to the unsigned Laplacians in paths with initial states of the form e_a+e_b. That is, P_3, P_4 are the only paths where perfect state transfer relative to the unsigned Laplacians occurs and it occurs between the end-edges of P_3, P_4 at time $\pi/2$, $\sqrt{2}\pi/2$ respectively .

Notice also that P_2, P_3 are the line graphs of P_3, P_4 respectively. In P_3 and its line graph P_2, perfect state transfer always occurs at the same time $\pi/2$ between the same pair of edges and their corresponding pair of vertices in the line graph. This happens regardless of our choice of Hamiltonian or form of the initial state. We can make the same observations about perfect state transfer in P_4 ant its line graph P_3.

Notice that C_4 is the line graph of itself. An analogous comment can be made on perfect state transfer on cycles as well. We know that C_4 is the only cycle that admits perfect state transfer relative to adjacency matrices, Laplacians and unsigned Laplacians. No matter our choice of Hamiltonians and form of initial state, perfect state transfer happens at the same time $\pi/2$ between pairs of opposite edges or vertices. Since cycles are regular graphs, the transition matrices relative to adjacency matrices, Laplacians and unsigned Laplacians are all equivalent up to some phase factor. It is still surprising that different forms of initial states: $e_a, e_a - e_b$ or $e_a + e_b$ actually do not affect perfect state transfer in C_4.

It seems that there is a correspondence between perfect edge state transfer in a graph and perfect vertex state transfer in its line graph. However, that is not true for most graphs. So far, paths and cycles are the only examples we have found where the correspondence can be observed. The author does not know yet the cause behind the correspondence.

Chapter 6

Unsigned Laplacian

As mentioned in Section 2.2, the unsigned Laplacian of a graph is also a legitimate choice for Hamiltonian of a quantum walk. When the unsigned Laplacian of a graph is used as Hamiltonian of the overlying quantum walk, we characterize perfect state transfer on three class of graphs: bipartite graphs, cycles and paths. Throughout this section, if G is a graph, then $A(G), \Delta(G)$ denote the adjacency matrix and degree matrix of G respectively.

Let G be a graph. The *unsigned Laplacian* of G is matrix $L_+(G)$ such that

$$L_+(G) = \Delta(G) + A(G).$$

When we use $L_+(G)$ as Hamiltonian in a quantum walk, the edge (a, b) of G is associated with the state

$$e_a + e_b,$$

which we call "*plus state*".

Since the main case of interest in this thesis is the case when the Laplacian of a graph is used as Hamiltonian, it is natural to question if there will be perfect state transfer between a edge state and a plus state when we use the Laplacian as Hamiltonian. The answer is no.

6.0.1 Theorem. *Let G be a graph with $a, b, c, d \in V(G)$. There is no perfect state transfer between a state of the form $e_a + e_b$ and a state of the form $e_c - e_d$ in G when the Laplacian of G is used as Hamiltonian of the quantum walk.*

Proof. We know that 0 will always be a eigenvalue of the Laplacian of G with the all-ones vector being its eigenvector. Thus, we know 0 will never be in the eigenvalue support of $e_a - e_b$ while 0 is always in the eigenvalue support of $e_c + e_d$. It follows that $e_a - e_b$ and $e_c + e_d$ do not have the same eigenvalue support, which implies that they are not strongly cospectral. By Theorem 2.6.1, we can conclude that there is no perfect state transfer between a state of the form $(e_a - e_b)$ and a state of the form $(e_c + e_d)$ using Laplacian as Hamiltonian. □

Every time we refer to plus states, we use the unsigned Laplacian of a graph as Hamiltonian unless stated explicitly otherwise. We define analogously that there is *perfect plus state transfer* between $e_a + e_b$ and $e_c + e_d$ if and only if

$$U(t)(e_a + e_b) = \exp(itL_+)(e_a + e_b) = \gamma(e_c + e_d),$$

for some complex constant γ. Also, a plus state $e_a + e_b$ is periodic if and only if it has perfect plus state transfer to itself at some time t.

6.1 Bipartite Graphs

When the underlying graph of a quantum walk is a bipartite graph, using the signed or unsigned Laplacian as Hamiltonian is essentially the same. This is due to that the Laplacian and unsigned Laplacian of a bipartite graph are similar. In this section, all the results related to quantum state transfer are due to the author.

6.1.1 Lemma. *Let G be a bipartite graph with two parts B_1, B_2 and A, Δ denote the adjacency matrix and the degree matrix of G respectively. Let D be block matrix such that*

$$D = \begin{pmatrix} -I & \mathbf{0} \\ \mathbf{0} & I \end{pmatrix}$$

indexed by the vertices of B_1, B_2 in the order . Then we have

$$D(\Delta - A)D = \Delta + A.$$

Proof. Since G is a bipartite, we know that A is in the form of

$$\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix},$$

where the rows are indexed by the vertices in B_1, B_2 in order. Then we have that
$$DAD = -A.$$
Since $D\Delta D = \Delta$, we have that
$$D(\Delta - A)D = \Delta + A. \qquad \square$$

6.1.2 Theorem. *Let G be a bipartite graph with parts B_1, B_2 and vertices $a, c \in B_1$ and $b, d \in B_2$. There is perfect edge state transfer between $(e_a - e_b)$ and $(e_c - e_d)$ if and only if there is perfect plus state transfer between $(e_a + e_b)$ and $(e_c + e_d)$.*

Proof. Let Δ denote the degree matrix of G and A denote the adjacency matrix of G. From the Lemma 6.1.1, we know that
$$D(\Delta - A)D = \Delta + A$$
and inserting $DD = I$ between m copies of $\Delta - A$, we have
$$\begin{aligned} D(\Delta - A)^m D &= D(\Delta - A)DD(\Delta - A)DD \cdots (\Delta - A)D \\ &= (\Delta + A)^m \end{aligned}$$
for any non-negative integer m. Then we see that
$$\begin{aligned} DU(t)D = D\exp(itL)D &= D\sum_{m=0}^{\infty}\left(\frac{(it)^m}{m!}(\Delta - A)^m\right)D \\ &= \sum_{m=0}^{\infty}\frac{(it)^m}{m!}D(\Delta - A)^m D \\ &= \sum_{m=0}^{\infty}\frac{(it)^m}{m!}(\Delta + A)^m \\ &= \exp(itL_+) \end{aligned}$$
Note that since $a, c \in B_1$ and $b, d \in B_2$, we have that
$$D(e_a - e_b)D = -(e_a + e_b), \quad D(e_c - e_d)D = -(e_c + e_d).$$

There is perfect state transfer between $(e_a - e_b)$ and $(e_c - e_d)$ using Laplacian if and only if there exist τ such that

$$U(\tau)(e_a - e_b) = \gamma(e_c - e_d)$$

for some $|\gamma| = 1$. Applying D on both sides of the equation above, we have that

$$DU(\tau)(e_a - e_b) = D\left(\gamma(e_c - e_d)\right).$$

Again using $DD = I$, we can rewrite the equation above as

$$DU(\tau)DD(e_a - e_b) = \gamma D(e_c - e_d).$$

This gives us that

$$-\exp(i\tau L_+)(e_a + e_b) = -\gamma(e_c + e_d),$$

$$\exp(i\tau L_+)(e_a + e_b) = \gamma(e_c + e_d),$$

which is equivalent to perfect plus state transfer between $(e_a + e_b)$ and $(e_c + e_d)$ using unsigned Laplacian. This completes our proof. □

6.2 Cycles and Paths

The argument used in the proof of Lemma 5.3.2 works for unsigned Laplacian of C_n as well, which gives us the next lemma.

6.2.1 Lemma. *Unsigned Laplacian eigenvectors of C_n are*

$$v_k = \begin{pmatrix} 1 \\ \omega^k \\ \omega^{2k} \\ \omega^{3k} \\ \vdots \\ \omega^{(n-1)k} \end{pmatrix}$$

for $k = 0, 1, \cdots, n-1$ where $\omega = e^{\frac{2\pi}{n}i}$ with eigenvalues

$$2 + 2\cos\frac{2\pi k}{n}$$

for $k = 0, 1, \cdots, n-1$. □

Notice that all-ones vector is always an unsigned Laplacian eigenvector of C_n with eigenvalue 4. By the proof of Lemma 5.3.3, we know that when n is even, the unsigned Laplacian of C_n has $1 + \frac{n}{2}$ distinct eigenvalues while when n is odd, it has $\lceil \frac{n}{2} \rceil$ distinct eigenvalues. But n is even if and only if the unsigned Laplacian of C_n has eignvalue 0 and its corresponding eigenvector

$$\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \\ \vdots \\ 1 \\ -1 \end{pmatrix}$$

with the alternating signs of entries. Thus, we can see that 0 cannot be in the eigenvalue support of a plus state when n is even. Therefore, we get the following lemma.

6.2.2 Lemma. *Every plus state of C_n has unsigned Laplacian eigenvalue support of size $\lceil \frac{n}{2} \rceil$.* □

Like perfect edge state transfer, periodicity of an edge state is required for the state to have perfect plus state transfer.

6.2.3 Theorem. *There is perfect plus state transfer in C_n if and only if $n = 4$.*

Proof. By Lemma 6.2.1, the unsigned Laplacian eigenvalues of C_n are

$$0 \leq 2 + 2\cos\frac{2\pi k}{n} \leq 4$$

for $k = 0, 1, \cdots, n-1$. By Corollary 3.2.8, we know that for a plus state to be periodic, the size of eigenvalue support must be at most 4. Then by Lemma 6.2.2, if C_n has a periodic plus state, then $3 \leq n \leq 8$.

Using Theorem 3.2.7, we can find that there are no periodic plus states in C_n when $n = 5, 7, 8$ which implies that there is no perfect edge state transfer in C_n. Since cycles are edge-transitive, by Corollary 3.4.8, we know there is no perfect state transfer in C_3. Computing

$$\left| \frac{1}{2}(e_a + e_b)^T U(t)(e_c + e_d) \right|^2$$

for all distinct edges $(a, b), (c, d)$ in $E(C_n)$ when $n = 4, 6$, we can conclude that the only cycle that has perfect plus state transfer is C_4. □

In C_4, there is perfect plus state transfer between opposite edges at time $\frac{\pi}{2}$. This can also be viewed as a consequence of Theorem 6.1.2 due to the fact that C_4 is a bipartite graph.

Note that the unsigned Laplacian of a graph G shares a strong correspondence with the line graph of G via the incidence matrix of G. To understand the spectral properties of the unsigned Laplacian of paths, we first introdue the incidence matrices.The *incidence matrix* B of a graph G is a $|V(G)| \times |E(G)|$ matrix whose rows and columns are indexed by vertices and edges of G respectively such that

$$B_{ij} = \begin{cases} 1 & \text{if vertex } i \text{ is an end of edge } j, \\ 0 & \text{otherwise.} \end{cases}$$

Then we know that

$$BB^T = A(G) + \Delta(G), \quad B^T B = A(G') + 2I,$$

where G' is the line graph of G.

Using the standard result from linear algebra fact stated below, we can easily figure out the eigenvalues of the unsigned Laplacian of P_n.

6.2.4 Lemma. *Let M be a square matrix. Then M and M^T have the same eigenvalues with the same multiplicities.* □

6.2.5 Corollary. *The unsigned Laplacian eigenvalues of P_n are*

$$2 + 2\cos\frac{\pi r}{n}$$

for $r = 0, 1, \cdots, n-1$.

Proof. Notice that the line graph of P_n is the path P_{n-1}. Let B be the incidence matrix of P_n. Then we have that

$$B^T B = 2I + A(P_{n-1}), \quad BB^T = \Delta + A(P_n).$$

By previous lemma, we know that $A(P_n) + \Delta(P_n)$ and $A(P_{n-1}) + 2I$ have the same eigenvalues, that is,

$$2 + 2\cos\frac{\pi r}{n}$$

for $r = 0, 1, \cdots, n-1$. □

Let z be a Laplacian eigenvector of P_n with eigenvalue θ. Then by changing the sign of the entries of z indexed by a color class, we obtain an eigenvector for the unsigned Laplacian of P_n with the same eigenvalue θ. From this, we can get the following theorem.

6.2.6 Theorem. *Let (a, b) be an edge in P_n. Then the eigenvalue supports of $e_a - e_b$ and $e_a + e_b$ are the same.* □

6.2.7 Theorem. *A path graph on n vertices has perfect plus state transfer if and only if $n = 3, 4$.*

Proof. By Theorem 6.2.2, we know that the plus state and the edge state associated with an edge of P_n have the same eigenvalue support, which implies an analogous version of Lemma 5.4.6 for plus states. That is, the size of eigenvalue supports of a plus state in P_n must be at least $\frac{n}{2}$. By Corollary 6.2.5, we know that the unsigned Laplacian eigenvalues of P_n are

$$0 \leq 2 + 2\cos\frac{\pi r}{n} \leq 4$$

for $r = 0, 1, \cdots, n-1$.

By Corollary 3.2.8, we know that if a plus state of P_n is periodic, then its eigenvalue support has size at most four. Since the size of a plus state in P_n is at least $\frac{n}{2}$, there is no periodic plus state in P_n for $n \geq 9$. Since periodicity is a necessary condition for a plus state to have perfect state transfer, there is no perfect plus state transfer in P_n for $n \geq 9$.

Using Theorem 3.2.7 we find that when $n = 5, 7, 8, 9$, there are no periodic plus states in P_n and also that there is only one periodic plus state in P_6. If the vertices of P_6 from one end to the other are $0, 1, \cdots, 5$, then $e_2 - e_3$ is the only periodic state with period $2\sqrt{3}\pi/3$. Thus, we can conclude that when $n = 5, 6, 7, 8, 9$, there is no perfect plus state transfer in P_n.

By computing

$$\left| \frac{1}{2}(e_a + e_b)^T U(t)(e_c + e_d) \right|^2$$

for all distinct edges $(a, b), (c, d)$ in $E(P_3)$ and $E(P_4)$, we find that there is perfect state transfer in P_3 and P_4. Therefore, there is perfect plus state transfer in P_n if and only if $n = 3, 4$. □

Perfect edge state transfer and perfect plus state transfer happen between the same pairs of edges at the same time in P_3 and P_4. When $n = 3$, there is perfect plus state transfer between its edges in P_3 at time $\pi/2$. When $n = 4$, perfect plus state transfer occurs between two edges on its ends in P_4 at time $\sqrt{2}\pi/2$.

6.3 Comparison with the Laplacian

G_n	total	Lap. PED	Lap. PST	Unsigned PED	Unsigned PST
G_5	21	18 (85.7%)	6 (28.6%)	4 (19.0%)	0 (0%)
G_6	112	86 (76.8%)	25 (22.3%)	21 (18.8%)	4 (3.6%)
G_7	853	513 (60.1%)	94 (11.0%)	23 (2.7%)	2 (0.2%)
G_8	11117	5164 (46.5%)	673 (6.0%)	55 (0.5%)	14 (0.1%)

Table 6.1: the Number of Graphs with PST and Periodic States

In Table 6.1, we use G_n denote the set of connected graphs on n vertices and the second column show the cardinality of G_n. The column "Lap. PED" shows the number of graphs in G_n that have periodic edge states and its proportion. The column "Lap. PST" shows the number of graphs in G_n that have perfect edge state transfer and its proportion. The column "Unsigned PED" shows the number of graphs in G_n that have periodic plus states and its proportion. The column "Unsigned PST" shows the number of graphs in G_n that have perfect plus state transfer and its proportion.

In a regular graph G with valency k, we have that

$$L(G) = A(G) - kI, \quad L_+(G) = A(G) + kI.$$

Thus, we can see that the transition matrices of a quantum walk on a regular graph with respect to the adjacency matrix, the Laplacian and the unsigned Laplacian are equivalent up to some phase factor.

Apart from the cases when underlying graphs of quantum walks are regular, from the table above, we can see that there is a huge difference between the number of periodic edge states relative to the Laplacians and periodic plus states relative to the unsigned Laplacians in general. This contributes to the huge gap between the number of perfect edge state transfer and the number of perfect plus state transfer.

In terms of quantum walks, one significant difference between the Laplacians and the unsigned Laplacians is that zero can be a legitimate candidate as an eigenvalue in the eigenvalue supports of a plus state but can never be in the eigenvalue support of an edge state. However, our studies on quantum walks relative to the unsigned Laplacian are still at an early stage and we have not found causes for those huge gaps.

Chapter 7

Open Questions

Regardless of Hamiltonians and initial states, perfect state transfer is significant but rare in quantum communication. So we always try to find more graphs with perfect state transfer. Along this line, we raise three main questions in this chapter.

7.1 Hamiltonians and Initial States

In this thesis, we mainly focus on the case when the Hamiltonian is the Laplacian of the underlying graph of a quantum walk and the initial state is in the form of

$$e_a - e_b.$$

But as mentioned briefly in Section 2.2, the most investigated case so far is the case when the adjacency matrix of a graph is used as Hamiltonian with vertex states as the initial states. Coutinho and Liu prove that there is no Laplacian perfect vertex state transfer in trees with more than two vertices in [9]. Alvir et al. [1] also studies vertex state transfer relative to Laplacians, unsigned Laplacians and normalized Laplacians. They observed that complementation preserves Laplacian perfect vertex state transfer. They also proved that under certain spectral condition, the weak product of graphs preserves perfect vertex state transfer relative to normalized Laplacian.

G_n	Total	$A(G_n)$ with vertex states	Prop.	$L(G_n)$ with edge states	Prop.	$L_+(G_n)$ with plus states	Prop.
G_5	21	7	33.3%	18	61.9%	4	19.0%
G_6	112	10	8.9%	86	44.6%	21	18.76%
G_7	853	23	2.7%	513	22.4%	23	2.7%
G_8	11117	40	0.4%	673	11.4%	55	0.5%

Table 7.1: Periodic States in Different Hamiltonians with Different Forms of Initial States

Table 7.1 shows that the number of graphs with adjacency periodic vertex states, Laplacian periodic edge states and unsigned Laplacian periodic plus states followed with the corresponding proportions from left to right in order.

From Table 7.1 as well as Table 2.1, we can see that different choices of Hamiltonian and different forms of initial state largely affect the number of periodic states in a graph and hence, affect the number of states that have perfect state transfer.

However, as shown in Chapter 5 and Chapter 6, when we consider perfect state transfer in paths and cycles, using the Laplacian as Hamiltonian with edges states as initial states gives us the same result as using the unsigned Laplacian as Hamiltonian with plus states as initial states. We can see that perfect state transfer in some certain classes of graphs is invariant under different Hamiltonians and initial states.

Given a specific graph, we are curious about how to choose Hamiltonian and the initial state so that the quantum walk over the graph will have desired phenomena, such as perfect state transfer between some certain pairs. On the other hand, given Hamiltonian and specific initial state, we would like to know how one can construct a graph with perfect state transfer. Also, we would like to know what conditions a graph has to satisfy to admit ”stable” perfect state transfer under different Hamiltonians and different forms of initial states.

7.2 Constructions

In Chapter 4, we provide two ways to construct new graphs with perfect edge state transfer based on some given graphs with perfect edge state transfer. We would like to find more ways to construct new graphs that admit perfect edge state transfer.

One possible graph operation the author briefly looked into is taking strong product of two graphs. The *strong product* $G \boxtimes H$ of two graphs G and H is a graph with vertex set $V(G) \times V(H)$. Two distinct vertices (g_1, h_1) and (g_2, h_2) are adjacent in $G \boxtimes H$ if g_1 is equal or adjacent to g_2 in G, and h_1 is equal or adjacent to h_2 in H. To understand the strong product of two graphs better, we introduce the direct product of two graphs.

Let $G \times H$ denote the *direct product* of G and H that is a graph with vertex set $V(G) \times V(H)$. Two distinct vertices (g_1, h_1) and (g_2, h_2) are adjacent in $G \times H$ if and only if g_1 is adjacent to g_2 in G, and h_1 is adjacent to h_2 in H.

Note that the strong product of G and H can be viewed as the union of the Cartesian product and the direct product of G and H. We can write the transition matrix on $G \boxtimes H$ in terms of the transition matrix on $G \times H$ and the transition matrix $G \square H$.

7.2.1 Lemma. *Let G, H be two graphs and $G \boxtimes H$ denotes the strong product of G and H. Then*

$$U_{G \boxtimes H}(t) = U_{G \square H}(t) U_{G \times H}(t).$$

Proof. If X is a graph, we use $A(X)$ and $\Delta(X)$ to denote the adjacency matrix and the degree matrix of X respectively. Also, we use $L(X)$ to denote the Laplacian matrix of X. By the construction of strong product of G and H, it is easy to see that

$$A(G \boxtimes H) = A(G \square H) + A(G \times H)$$

and

$$\Delta(G \boxtimes H) = \Delta(G \square H) + \Delta(G \times H).$$

Then we can have that

$$\begin{aligned} L(G \boxtimes H) &= \Delta(G \boxtimes H) - A(G \boxtimes H) \\ &= \Delta(G \square H) + \Delta(G \times H) - (A(G \square H) + A(G \times H)) \\ &= L(G \square H) + L(G \times H). \end{aligned}$$

It follows that

$$\begin{aligned} U_{G\boxtimes H}(t) &= \exp\left(itL(G\boxtimes H)\right) \\ &= \exp\left(it\left(L(G\Box H) + L(G\times H)\right)\right) \\ &= \exp\left(itL(G\Box H)\right)\exp\left(itL(G\times H)\right) \\ &= U_{G\Box H}(t)\cdot U_{G\times H}(t), \end{aligned}$$

which completes our proof. □

Let (a, b) be an edge of $G\boxtimes H$. From the lemma above, we can see that if $e_a - e_b$ has perfect state transfer with $e_c - e_d$ in $G \times H$ at time τ and there is perfect state transfer from $e_c - e_d$ to $e_f - e_g$ in $G\Box H$ at time τ, then there is perfect state transfer between $e_a - e_b$ and $e_f - e_g$ in $G\boxtimes H$ at time τ. This theory works perfectly for some examples, such as perfect edges state transfer occurring in $P_2 \boxtimes C_4$. However, there are some examples for which this theory does not work, such as $P_2 \boxtimes P_3$.

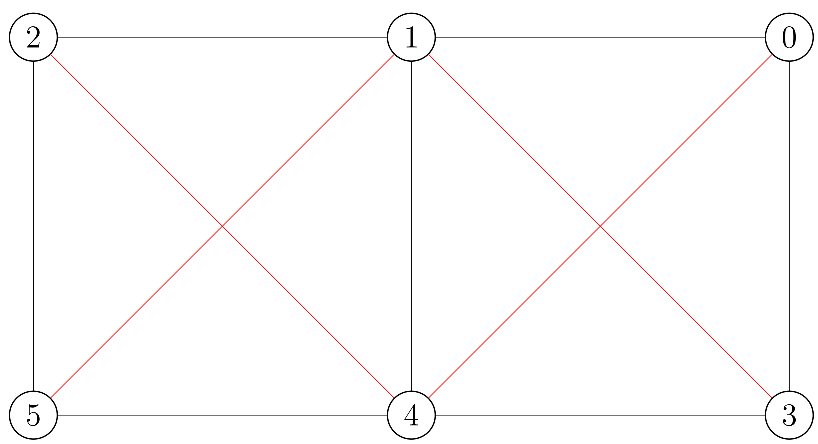

Figure 7.1: $P_2 \boxtimes P_3$

Notice that

$$E(P_2 \boxtimes P_3) = E(P_2 \times P_3) \cup E(P_2 \Box P_3)$$

and the red edges of the graph in Figure 7.1 are in $E(P_2 \times P_3)$ while the black edges are in $E(P_2 \Box P_3)$.

Calculations in `SAGE` show that there is perfect edge state transfer in $P_2 \boxtimes P_3$ between edges states associated with the following four pairs of edges at time $\frac{\pi}{2}$:

- $(1,0),(1,3)$,
- $(4,0),(4,3)$,
- $(1,2),(1,5)$,
- $(4,2),(4,5)$.

In Section 4.2, we show that there is perfect edge state transfer in $P_2 \square P_3$ (Figure 4.1) between edge states associated with the following two pairs of edges at time $\frac{\pi}{2}$:

- $(1,2),(3,4)$,
- $(1,0),(4,5)$.

We can see that $P_2 \times P_3$ is disjoint union of two paths on three vertices. As proved in Section 5.4, there is only perfect state transfer between edges states associated with the following two pairs of edges at time $\frac{\pi}{2}$:

- $(2,4),(0,4)$,
- $(1,5),(1,3)$

and there is no perfect edge state transfer in the complement of $P_2 \times P_3$. The author has not been able to explain what contributes to perfect edge state transfer between those four pairs in $P_2 \boxtimes P_3$.

So far, all the ways to construct new graphs admitting perfect edge state transfer are based on some known graphs with perfect edge state transfer. We would also like to know what kind of graphs can admit perfect edge state transfer, which leads us to the next section.

7.3 Characterizations

In [7, Section 7.3], Coutinho states the sufficient and necessary conditions for Laplacian perfect vertex state transfer to occur. The eigenvalue support of e_u is denoted by Λ_u. If u and v are strongly cospectral with respect to the Laplacian $\sum_r \lambda_r F_r$, then $\Lambda_u = \Lambda_v$. For strongly cospectral vertices u, v, define the partition $\{\Lambda_{uv}^+, \Lambda_{uv}^-\}$ of $\Lambda_u = \Lambda_v$ such that

$$\lambda_r \in \Lambda_{uv}^+ \iff F_r e_u = F_r e_v, \quad \lambda_r \in \Lambda_{uv}^- \iff F_r e_u = -F_r e_v.$$

7.3.1 Theorem. *Let X be a graph, $u, v \in V(X)$. Let $\lambda_0 > \cdots > \lambda_k$ be the eigenvalues in Λ_u. Then X admits perfect state transfer with respect to the Laplacian from u to v at time τ with phase γ if and only if all of the following conditions hold.*

(i) Vertices u and v are strongly cospectral with respect to the Laplacian.

(ii) Elements in Λ_u are all integers.

(iii) Let $g = \gcd\left(\{\lambda_r\}_{r=0}^{k}\right)$. Then

(a) $\lambda_r \in \Lambda_{uv}^{+}$ if and only if $\frac{\lambda_r}{g}$ is even, and

(b) $\lambda_r \in \Lambda_{uv}^{-}$ if and only if $\frac{\lambda_r}{g}$ is odd. □

By the theorem above, we can see that whether a graph admits Laplacian perfect vertex state transfer can only depend on spectral properties of the Laplacian of the graph.

We wonder if the spectra of the Laplacian of a graph can determine perfect edge state transfer on the graph. Also, we are curious about what kind of graphs can have those spectral properties and if there is a way to classify those graphs.

Glossary

$A(G)$	adjacency matrix of G. 2
C_n	cycle with n vertices. 62
$E(G)$	the set of all the edges of G. 3
$G \square H$	Cartesian product of G and H. 49
$G \boxtimes H$	strong product of G and H. 91
$G \times H$	direct product of G and H. 91
J	all-ones matrix. 45
K_n	complete graph on n vertices. 48
$K_{m,n}$	complete bipartite graph. 59
$L(G)$	Laplacian matrix of G. 17
$L_+(G)$	unsigned Laplacian matrix of G. 79
$M \circ N$	schur product of M and N. 8
P_n	path with n vertices. 68
$V(G)$	the set of all the vertices of G. 9
$\Delta(G)$	degree matrix of G. 2
$\mathrm{Aut}(G)$	automorphism of G. 23
$\mathrm{Col}(A)$	column space of A. 23
$\overline{G}$	the complement of graph G. 45
$\deg(i)$	degree of vertex i. 2
$\mathrm{rk}\, D$	rank of matrix D. 27
e_v	v-th standard basis vector. 3

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Index