Bipartite Quantum Walks and the Hamiltonian

by

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Author's Declaration

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.

I understand that my thesis may be made electronically available to the public.

Abstract

We study a discrete quantum walk model called bipartite walks via a spectral approach. A bipartite walk is determined by a unitary matrix U, i.e., the transition matrix of the walk. For every transition matrix U, there is a Hamiltonian H such that $U = \exp(iH)$. If there is a real skew-symmetric matrix S such that $H = iS$, we say there is a H-digraph associated to the walk and S is the skew-adjacency matrix of the H-digraph. The underlying unweighted non-oriented graph of the H-digraph is H-graph. Let G be a simple bipartite graph with no isolated vertices. The bipartite walk on G is the same as the continuous walk on the H-digraph over integer time. Two questions lie in the centre of this thesis are

1. Is there a connection between the H-(di)graph and the underlying graph G? If there is, what is the connection?

2. Is there a connection between the walk and the underlying graph G? If there is, what is the connection?

Given a bipartite walk on G, we show that the underlying bipartite graph G determines the existence of the H-graph. If G is biregular, the spectrum of G determines the spectrum of U.

We give complete characterizations of bipartite walks on paths and even cycles. Given a path or an even cycle, the transition matrix of the bipartite walk is a permutation matrix. The H-digraph is an oriented weighted complete graph. Using bipartite walks on even paths, we construct a infinite family of oriented weighted complete graphs such that continuous walks defined on them have universal perfect state transfer, which is an interesting but rare phenomenon.

Grover's walk is one of the most studied discrete quantum walk model and it can be used to implement the famous Grover's algorithm. We show that Grover's walk is actually a special case of bipartite walks. Moreover, given a bipartite graph G, one step of the bipartite walk on G is the same as two steps of Grover's walk on the same graph.

We also study periodic bipartite walks. Using results from algebraic number theory, we give a characterization of periodic walks on a biregular graph with a constraint on its spectrum. This characterization only depends on the spectrum of the underlying graph and the possible spectrum for a periodic walk is determined by the degrees of the underlying graph. We

apply this characterization of periodic bipartite walk to Grover's walk to get a characterization of a certain class of periodic Grover's walk.

Lastly, we look into bipartite walks on the incidence graphs of incidence structures, t-designs ($t \geq 2$) and generalized quadrangles in particular. Given a bipartite walk on a t-design, we show that if the underlying design is a partial linear space, the H-graph is the distance-two graph of the line graph of the underlying incidence graph. Given a bipartite walk on the incidence graph of a generalized quadrangle, we show that there is a homogeneous coherent algebra raised from the bipartite walk. This homogeneous coherent algebra is useful in analyzing the behavior of the walk.

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Although the importance of the individuals mentioned in this section are not ranked in descending order, I would like to say my supervisor, Chris Godsil, is the most important person in my six-year journey. I would like to thank him for his unwavering support, believing in me even at times when I did not, and for always having the right answers to my questions, math and otherwise. He has shown me how to be a better researcher, and even more importantly, how to be a better person.

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I would not be where I am without my parents. Mom, who apparently I inherit my sense of humor from, thank you for your constant, sometimes blind, optimism. Dad, who values my education over anything else, thank you for all the sacrifices you made.

According to Matthew Hough, a good acknowledgement should not be over a page. But that would mean that I have to cut him out. Given that he most likely is going to be the only person who voluntarily reads through my thesis word by word, I decide to risk it.

Matt, thank you for all the butterflies and coffee beans.

I am extremely grateful for ALL the people I met here in Waterloo. I hope one day I will be able to pass on the kindness and love I received here.

Dedication

This is dedicated to my parents.
(献给我的父母：陈黎明， 吴凤霞。)

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Chapter 1

Introduction

Quantum walks, as the quantum analogues of classical random walks, are powerful tools for quantum computing [10] and developing quantum algorithms [11, 26, 34].

Depending on how the system evolves, there are two classes of quantum walks: continuous quantum walk and discrete quantum walks. In a continuous quantum walk, the state of the walker is evolving constantly, while in a discrete quantum walk, a system evolves in a discrete steps and in each step the walker performs an operation that updates her state. For the purpose of this thesis, a quantum walk (continuous or discrete) is described by a unitary matrix, which we call the transition matrix of the walk.

Given a graph G, the transition matrices of a continuous quantum walk are of the form

$$U(t) := \exp(itH), \quad (t \in \mathbb{R}),$$

where H is usually either the adjacency matrix or, less often, the Laplacian of G. Given a unit vector x_0 as its initial state, the system of a continuous quantum walk at time t is at the state

$$U(t)x_0.$$

Equivalently, if the initial state is given as a density matrix D_0, then the state of the system at time t is

$$U(t)D_0U(-t).$$

Consequently, the spectrum of the underlying graph determines the behavior of the continuous walk and there have been many studies done [12,15,16].

In contrast, there is no obvious connection between the behavor of a discrete quantum walk and its underlying graph.

In most discrete quantum walk models, the transition matrix of a discrete quantum walk can be written as a product of two unitary matrices, i.e.,

$$U = U_1 U_2.$$

Given a unit vector x_0 as its initial state, the system of a discrete quantum walk at k-th step will be at the state

$$U^k x_0.$$

Equivalently, if the initial state is given as a density matrix D_0, then the state of the system at k-th step is

$$U^k D_0 U^{-k}.$$

It is possible that U_1, U_2 depend on the underlying graph. But in general, matrices U_1, U_2 do not commute, which means spectra of U_1, U_2 do not affect the spectrum of U directly.

The question lies in the centre of this thesis is how the underlying graph affects the discrete quantum walk defined on it. To explore this, the model we study is bipartite walks.

We provide a brief description of a bipartite walk. Given a bipartite graph G, we assume that X and Y are the two colour classes of G and using these we construct two partitions of $E(G)$. For the first partition, π_0, two edges are in the same cell if they have a vertex in common, and that vertex is in X. For the second partition π_1, two edges are in the same cell if they have a vertex in common, and that vertex is in Y. Each of these partitions determines a projection, namely the projection onto the functions on $E(G)$ that are constant on the cells of π_0 and π_1. We denote these projections by P and Q respectively. Then $2P - I$ and $2Q - I$ are unitary. (Geometrically they are reflections.) We define the transition matrix of the bipartite walk on G by

$$U := (2P - I)(2Q - I).$$

1.1 Bipartite walks in earlier literature

Given a graph, there are many different ways to define a discrete quantum walks on it [27,32,38]. The model we study in this thesis is bipartite walks.

For the purpose of this thesis, here we introduce two models that have connections to the bipartite walks of our interest.

Szegedy introduced the model of bipartite walks in [34]. Using a bipartite walk to quantize a Markov chain, Szegedy requires two parts of the underlying bipartite graph to have the same size. Our bipartite walks do not require this.

Later in [28], Konno et al. propose a discrete walk model: the two-partition model. This model includes bipartite walks we are going to study. They show that many well-studied discrete quantum walk models can be viewed as bipartite walks. This gives us more motivation to study bipartite walks.

Although bipartite walks have been in literature for a while, there is not much we can say about their Hamiltonians or the relation between the walk and the underlying bipartite graph. These are what we set out to study in this thesis.

Szegedy's model

In this section, we follow the terminology introduced in [31, Section 11.1, 11.2].

A classical discrete-time stochastic process is a sequence of random variables $\{X_t : t \in \mathbb{N}\}$, where X_t is the state of the stochastic process at time t and X_0 is the initial state. The state space $\mathcal{S}$ is discrete here, i.e., $\mathcal{S} = \mathbb{N}$. A *Markov chain* is a stochastic process, whose future state depends only on the present state, i.e.,

$$\mathrm{Prob}(X_{t+1} = j | X_t = i, X_{t-1} = i_{n-1}, \cdots, X_0\} = \mathrm{Prob}(X_{t+1} = j | X_t = i),$$

for all $t \geq 0$ and $i_0, i_1, \cdots, i, j \in \mathcal{S}$.

The idea of bipartite walks we are going to focus on this thesis originated in [34]. In that paper, Szegedy introduces bipartite walks as a quantization of a Markov chain.

Any time-independent Markov chain can be viewed as a directed graph with vertex set V and arc set $\mathcal{A}$. Define $p_{i,j} = \mathrm{Prob}(X_{t+1} = j | X_t = i)$. Arc (i, j) is in $\mathcal{A}$ if and only if $p_{i,j} > 0$. Given a Markov chain, Szegedy's model is defined on the bipartite digraph obtained by duplicating the directed graph that associated with the Markov chain. Note that since the bipartite digraph obtained here is from duplication, two parts X, Y of the bipartite digraph have the same size. For every $x \in X$, we define

$$p_{x,y} = \frac{1}{\deg(x)}$$

and for every $y \in Y$, we define

$$q_{x,y} = \frac{1}{\deg(y)}.$$

For every $x \in X$, define state

$$|\phi_x\rangle = \sum_{y \in Y} \sqrt{p_{x,y}} |x\rangle |y\rangle$$

and similarly, for every $y \in Y$, define state

$$|\psi_y\rangle = \sum_{x \in X} \sqrt{q_{x,y}} |x\rangle |y\rangle,$$

where

$$\sum_{y \in Y} p_{x,y} = 1, \quad \sum_{x \in X} q_{x,y} = 1.$$

Define

$$R_1 := 2 \sum_{x \in X} |\phi_x\rangle\langle\phi_x| - I, \quad R_2 := 2 \sum_{y \in Y} |\psi_y\rangle\langle\psi_y| - I$$

and the transition matrix of Szegedy's model is

$$R_1 R_2.$$

A Markov chain is unbiased if it occurs on an undirected and unweighted graph, i.e.,

$$p_{x,y} = \begin{cases} \frac{1}{\deg(x)} & \text{if } x \sim y \\ 0 & \text{otherwise.} \end{cases}$$

If the Markov chain is unbiased, then Szegedy's model can be viewed as a special case of bipartite walks we are going to study in this thesis.

Since the bipartite graph used in Szegedy's model is obtained from duplication, two parts must have the same size. The bipartite walks we are going to study in this thesis can be defined on any bipartite graphs. In [34], Szegedy introduces this model to study the hitting time problem. For us, the main interest will be finding a connection between the underlying bipartite graph and the walk.

Two-partition model

In [28], Konno et al. propose a discrete walk model called "two-partition model", which includes bipartite walks that we study in this thesis. The framework of two-partition model is as follows.

Given a countable set Ω and two equivalence relations π_1, π_2 over Ω, the set Ω can be partitioned in two ways. Consequently, we have two partitions: Ω/π_1 and Ω/π_2.

The Hilbert space induced by Ω is

$$\ell^2(\Omega) = \{\varphi : \Omega \to \mathbb{C} \mid \sum_{\omega \in \Omega} |\varphi(\omega)|^2 < \infty\}.$$

with standard inner product.

Let C_i denote an element of Ω/π_1 and D_j denote an element of Ω/π_2. Define

$$\mathcal{C}_i = \operatorname{span}\{\delta_\omega | \ \omega \in C_i\}$$

and

$$\mathcal{D}_i = \operatorname{span}\{\delta_\omega | \ \omega \in D_i\},$$

where δ_ω is the character vector of ω, i.e., δ_ω is a 01-vector and the i-th entry of δ_ω is one if and only if $i = \omega$. Define a local operator $\widehat{E}_i$ on $\mathcal{C}_i$ as follows:

$$\langle \delta_{\omega'}, \widehat{E}_i \delta_\omega \rangle = 0$$

if ω or ω' not in C_i and the local operator $\widehat{F}_j$ is defined on $\mathcal{D}_j$ in the same fashion.

Let

$$\widehat{F} = \bigoplus_j \widehat{F}_j, \quad \widehat{E} = \bigoplus_i \widehat{E}_i$$

and the transition matrix of this model is

$$\widehat{F}\widehat{E}.$$

Let U_1, U_2 be the transition matrices of two different discrete quantum walk models $\mathcal{W}_1, \mathcal{W}_2$ acting on $\ell^2(\Omega_1)$, $\ell^2(\Omega_2)$ respectively. Let $\eta : \Omega_1 \to \Omega_2$ be an injection map and it has corresponding unitary map $M_\eta : \ell^2(\Omega_1) \to \ell^2(\eta(\Omega_1))$ such that $(M_\eta \psi)(a) = \psi(\eta^{-1}(a))$. If

$$U_1 = M_\eta^{-1} U_2 M_\eta,$$

we write $\mathcal{W}_1 \prec \mathcal{W}_2$. If we have both $\mathcal{W}_1 \prec \mathcal{W}_2$ and $\mathcal{W}_2 \prec \mathcal{W}_1$, then $\mathcal{W}_1 \cong \mathcal{W}_2$, i.e., we say $\mathcal{W}_1, \mathcal{W}_2$ are unitarily equivalent.

In [28], Konno et al. show the unitary equivalence relations between the quantum walk models under the framework of two-partition based quantum walk. For example, they show that bipartite walks and staggered walks described in Table 1.1 are equivalent.

2-Partition	Bipartite walks	Coined walks	Staggered walks
Ω	edge set of a bipartite multigraph with parts (X, Y)	arc set of a directed multigraph	vertex set of a 2-tessellable graph
π_1	X-ends of edges	tails of arcs	tessellation $\mathcal{T}_1$
π_2	Y-ends of edges	corresponding edges	tessellation $\mathcal{T}_2$

Table 1.1: Examples of two-partition quantum walks

Konno et al. in [28, Theorem 1] show that many well-studied discrete quantum walk models can be viewed as bipartite walks. This means that the information we get about bipartite walks can be also applied to other models.

1.2 Main results

The discrete quantum walk model we study in this thesis is bipartite walks. Recall that at the beginning of this chapter, we defined the transition matrix of the bipartite walk on G to be

$$U := (2P - I)(2Q - I).$$

For every unitary matrix U, there are Hermitian matrices H such that

$$U = \exp(iH).$$

The Hamiltonian of U is

$$H = -i \sum_r \log(e^{i\theta_r}) E_r = \sum_r \theta_r E_r,$$

where $-\pi < \theta_r \leq \pi$. If there exists a real skew-symmetric S such that the Hamiltonian of the walk can be written as

$$H = iS, \tag{1.2.1}$$

then S can be viewed as the skew-adjacency matrix of an oriented weighted graph. We refer to the oriented weighted graph as the H-digraph and the underlying unweighted non-oriented graph is the H-graph. The Hamiltonian and the H-(di)graph are the main interest of this thesis.

Quantum walks are described by their transition matrices, which in turn are described by their Hamiltonians. The Hamiltonian plays a crucial role in understanding the walk.

Recall that in a continuous walk, the transition matrix is

$$U(t) := \exp(itH), \quad (t \in \mathbb{R}),$$

where H is a Hermitian matrix associated with the underlying graph.

Given a discrete quantum walk governed by a unitary matrix U, if the Hamiltonian of U can be of the form 1.2.1, we can view the walk as a continuous walk on the H-digraph over integer time. On the other hand, if the transition matrix of a continuous walk is $U(t)$, then $U(1)$ is the transition matrix of the discrete walk. Thus, the Hamiltonians serve as bridges connecting discrete walks and continuous walks. This connection allows us to study continuous walks via discrete quantum walk and the other way around. This is why we care about the Hamiltonian and the H-digraph of bipartite walks.

Given a bipartite graph G, three main questions I aim to answer in this thesis are:

1. Is there a connection between G and the H-(di)graph?

2. Can structure of G affect the behavior of the bipartite walk defined on G?

3. Is there a family of bipartite graphs such that their bipartite walks will give affirmative answers to both of the questions above?

A short answer to our first question is yes. We show that the existence of the H-digraph, i.e. if the Hamiltonian can have the form 1.2.1, is determined by G.

1.2.1 Corollary (2.4.2)**.** *Let U be the transition matrix of the bipartite walk on a bipartite graph G. Then there exist a real skew-symmetric matrix S such that the Hamiltonian H of U is of the form $H = iS$ if and only if $A(G)$ is invertible.* □

Now we know G determines the existence of the H-(di)graph of the walk. We want to know how the structure of G affects the structure of the H-(di)graph. This question is better answered with examples. So we will be addressing this question when we answer the third question of the list.

Question two

As we demonstrated at the beginning of this chapter, unlike continuous walks, in most discrete quantum walk models, it is not obvious how the structure of the underlying graph affects the walk. But in bipartite walks, we are able to show that there are connections between the walk and the graph that it is defined on.

Given a bipartite graph G, let U be the transition matrix of the bipartite walk defined on G. We show that if G is biregular, we only need the spectrum of G or the spectrum of the line graph LG of G to determine the spectrum of U.

1.2.2 Theorem (5.3.1,2.5.1)**.** *Let G be a biregular graph with degree (d_0, d_1) and let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix of the bipartite walk defined on G. Then for every complex eigenvalue $e^{i\theta_r}$ of U, and for eigenvalue γ_r of $A(G)$, we have that*

$$\cos\theta_r = 2\frac{\gamma_r^2}{d_0 d_1} - 1. \tag{1.2.2}$$

For eigenvalue λ_r of $A(LG)$, we have that

$$\cos\theta_r = 2\Big(\frac{1}{d_0 d_1}\lambda_r^2 + \frac{4 - d_0 - d_1}{d_0 d_1}\lambda_r + \left(\frac{4 - 2d_0 - 2d_1}{d_0 d_1} + \frac{1}{2}\right)\Big). \tag{1.2.3}$$

□

One behavior of bipartite walks we study in this thesis is periodicity. We say a state D is periodic if there exist a positive integer k such that

$$U^k D U^{-k} = D,$$

i.e., after k steps, the walk returns to her initial state. If the spectral decomposition of U is $\sum_r e^{i\theta_r} E_r$, then the eigenvalue support of a state D is the set

$$\left\{ \left(e^{i\theta_r}, e^{i\theta_s}\right) : E_r D E_s \neq 0 \right\}.$$

1.2.3 Theorem (5.1.1)**.** *Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix of a bipartite walk. State D_a is periodic if and only if $\theta_r, \theta_s \in \mathbb{Q}\pi$ for all $(e^{i\theta_r}, e^{i\theta_s})$ in the eigenvalue support of D_a.*

We mainly focus on periodic walks, i.e.,

$$U^k = I$$

for some positive integer k. In other words, every state is periodic in a periodic walk. Algebraic number theory is the machinery we use. Given a biregular graph with a constraint on its spectrum, we give necessary and sufficient conditions on when the bipartite walk on it will be periodic.

1.2.4 Theorem (5.3.4)**.** *Let G be a biregular graph with degree (d_0, d_1). Assume that squares of eigenvalues λ_r of $A(G)$ are algebraic integers with degree at most two. The bipartite walk defined over G is periodic if and only if every eigenvalue λ_r of $A(G)$ satisfies that*

(a) if λ_r^2 is an algebraic integer of degree one, then $d_0 d_1 \equiv 0 \pmod 4$ and

$$\lambda_r^2 \in \left\{ \frac{1}{2} d_0 d_1,\ \frac{3}{4} d_0 d_1,\ \frac{1}{4} d_0 d_1,\ 0,\ d_0 d_1 \right\};$$

(b) if λ_r^2 is an algebraic integer of degree two, then

$$\lambda_r^2 \in \left\{ \left(\frac{1}{2} \pm \frac{\sqrt{2}}{4}\right) d_0 d_1,\ \left(\frac{1}{2} \pm \frac{\sqrt{3}}{4}\right) d_0 d_1,\ \frac{5 \pm \sqrt{5}}{8} d_0 d_1,\ \frac{3 \pm \sqrt{5}}{8} d_0 d_1 \right\}.$$

Moreover, λ_r^2 comes in algebraic conjugate pairs. □

This characterization depends only on the spectrum of the underlying biregular graph and the possible valid spectrum is determined solely by the degree of the biregular graph. So we can see in this case the underlying graph actually determines if the walk is periodic or not.

Using bipartite walks, we show that this connection between periodicity of the walk and the underlying graph also holds for another discrete quantum walk model: Grover's walk.

Grover's walk is one of the most studied discrete quantum walk model and it can be used to implement the famous Grover's search algorithm. We show that Grover's walk is a special case of bipartite walks. Not only that, we also show that if G is a bipartite graph, then every two steps of Grover's walk on G is equivalent to one step of bipartite walk on the same graph.

1.2.5 Theorem (4.4.1, 4.5.1)**.** *Given a graph G whose subdivision graph is denoted by $S(G)$, let $U_{BW}, U_{BW}(S(G))$ be the transition matrices of the bipartite walk defined on $G, S(G)$ respectively. Let $U_{GW}(G)$ be the transition matrix of Grover's walk defined on G. Then*

$$U_{BW}(S(G)) = U_{GW}(G).$$

Moreover, if G is a bipartite graph, for any non-negative integer k, we have that

$$U_{GW}(G)^{2k} = \begin{pmatrix} U_{BW}^k & 0 \\ 0 & {U_{BW}^T}^k \end{pmatrix}. \qquad \square$$

Using the correspondence between spectrum of a regular graph and that of its subdivision graph we proved in Corollary 5.4.3, we can apply the characterization above to give a characterization of periodic Grover's walks on regular graphs with a constraint on its spectrum.

1.2.6 Corollary (5.5.1)**.** *Let G be a d-regular graph, all of whose eigenvalues are algebraic integers of degree at most two in the form of*

$$\lambda_r = a + b\sqrt{m_r},$$

for some $a, b \in \mathbb{Q}$ and square-free integer m_r. The Grover's walk defined on G is periodic if and only if for every eigenvalue λ_r of G,

(a) *if $b = 0$, $\lambda_r \in \left\{0, \pm d, \pm\frac{1}{2}d\right\}$;*

(b) *if $b \neq 0$, $\lambda_r \in \left\{\pm\frac{\sqrt{2}}{2}d, \pm\frac{\sqrt{3}}{2}d, \frac{1\pm\sqrt{5}}{4}d, \frac{-1\pm\sqrt{5}}{4}d\right\}$.*

Note that eigenvalues of G come in algebraic conjugate pairs. $\square$

Our results in periodicity of Grover's walk on regular graphs extend the main results by Kubota [Theorem 3.3, Theorem 4.1 in [29]]. In addition to that, we are also able to show the following.

1.2.7 Corollary (5.5.3)**.** *Let G be a regular bipartite graph. Assume that the square of each eigenvalue of G is rational. Then the bipartite walk defined on G is periodic if and only if Grover's walk defined on G is periodic.*

Question three

To answer this question, I have looked into paths, even cycles and incidence graphs of incidence structures. They all give an affirmative answer to our question.

Two of the simplest classes of bipartite graphs are paths and even cycles. We are able to give a complete characterization of the bipartite walk on them and the H-digraphs associated with them.

1.2.8 Theorem. *3.1.1 The transition matrix of the bipartite walk on P_n is an $(n-1)$-cycle permutation whose cycle form is*

$$(e_0, e_1, e_3, \cdots, e_{n-4}, e_{n-2}, e_{n-3}, e_{n-5}, \cdots, e_2)$$

if n is odd and

$$(e_0, e_1, e_3, \cdots, e_{n-5}, e_{n-3}, e_{n-2}, e_{n-4}, \cdots, e_2)$$

if n is even.

Note that in the theorem below, we omit the case when $n \equiv 1 \pmod 4$. That is because for the purpose of this thesis, we can omit those cases without missing anything insightful or interesting.

1.2.9 Theorem (3.1.2,3.1.3)**.** *For an even $n \geq 4$, the H-digraph obtained from the bipartite walk on P_n is an oriented K_{n-1}. When $n \equiv 3 \pmod 4$, let H be the Hamiltonian of $U(P_n)^2$, then H-digraph is the weighted skew adjacency matrix of two copies of oriented $K_{\frac{n-1}{2}}$.*

As we stated before, the Hamiltonians bring continuous walks and discrete walks together. We can use bipartite walks to construct rare but interesting phenomena in continuous walks. One example is the corollary below. Using what we know about the bipartite walk on an even path, we are able to construct an infinite family of weighted oriented graphs such that the continuous walks define on them have universal perfect state transfer.

1.2.10 Corollary. *3.3.1 Let n be an even integer. Let s, t be distinct integer in $\{1, \cdots, n-1\}$. we define*

$$\alpha = \begin{cases} \frac{t-s}{2}, & \text{if both } s, t \text{ are even;} \\ \frac{s+t+1}{2} & \text{if } s \text{ is odd and } t \text{ is even;} \\ \frac{-t-s-1}{2}, & \text{if } s \text{ is even and } t \text{ is odd;} \\ \frac{s-t}{2}, & \text{if both } s, t \text{ are odd.} \end{cases}.$$

Let

$$w(s,t) = \frac{2}{n-1} \sum_{r=1}^{\frac{n}{2}-1} \frac{2\pi r}{(n-1)} \sin\left(\frac{2\pi r}{n-1}\alpha\right).$$

If $w(s,t) > 0$, we orient the edge $\{s,t\}$ from s to t and give it weight $w(s,t)$ and If $w(s,t) < 0$, we orient the edge $\{s,t\}$ from t to s and give it weight $-w(s,t)$ for all distinct $s, t \in \{1, \cdots, n-1\}$. Let $\overrightarrow{A}$ be the weighted skew-adjacency matrix of the resulting weighted oriented K_{n-1}. Then the continuous walk with transition matrix $\exp(iA)$ has universal perfect state transfer and every state will get transferred perfectly to any other state within time $t \leq n-1$. □

Besides paths and even cycles, we also look into bipartite walks on incidence structures, t-designs ($t \geq 2$) and generalized quadrangles in particular. A flag (x, B) of an incidence structure is a point-block pair such that the point x is contained in the block B. In those cases, the state space is the space of complex functions onto flags of the underlying incidence structure.

Consider the bipartite walk defined on a symmetric t-design $\mathcal{D}$ with $t \geq 2$ and parameters (v, b, k, r, λ_t). Let U be the transition matrix. If $\mathcal{D}$ is symmetric, the Hamiltonian of U can be written as

$$H = -\frac{2\theta i}{\sin(\theta) rk} A(\overrightarrow{H}),$$

where $A(\overrightarrow{H})$ is the adjacency matrix of the H-digraph. We can give a similar formula for the Hamiltonian of U^2 for a non-symmetric t-design.

In Corollary 6.4.2, we show that whether the design is symmetric or not, the H-digraph has constant weight on each of its arcs and the weight is determined by the parameters of the underlying design.

In general, we do not know much about the H-digraph, but in the case of t-design, many properties of the H-digraphs are determined by the underlying design and its incidence graph G:

1. [Theorem 6.4.3] The H-digraph is Eulerian with
$$\text{in-degree}(v) = \text{out-degree}(v) = (k-1)(r-\lambda_2)$$
for every vertex v;
2. [Corollary 6.4.4] the H-digraph is weakly connected if and only if it is strongly connected;
3. [Theorem 6.4.5, 6.4.6] if G has girth $2d \geq 6$, then H-graph has diameter two and girth d.

More surprisingly, there is actually a strong connection between the underlying graph G and the H-graph of the walk. We show that $A(H)$ is a polynomial in $A(LG_i)$, where LG_i is the i-th distance matrix of the line graph of the incidence graph G of $\mathcal{D}$. Moreover, the H-graph is exactly LG_2 when the underlying design is a symmetric partial linear design, i.e., its incidence graph has girth at least six.

1.2.11 Theorem (6.4.7,6.4.8)**.** *Let $\mathcal{D}$ be a symmetric t-design with $t \geq 2$. Let $A(H)$ denote the adjacency matrix of the H-graph. Then*
$$A(H) \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle.$$
Moreover, if a symmetric t-design $\mathcal{D}$ with $r, k \neq 4$, then $\mathcal{D}$ is a partial linear space if and only if
$$A(H) = A(LG_2).$$
□

We are also able to get some information about the behavior of the walk on t-design. One important matrix we use to study the walk is the average mixing matrix . Given a walk governed by $U = \sum_r e^{i\theta_r} E_r$, the average mixing matrix of U is
$$\widehat{M} = \lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} U^k \circ \overline{U^k}.$$

We show that if $\widehat{M}$ is the average mixing matrix of the bipartite walk on a symmetric design, then

(i) [Theorem 6.5.3] $\widehat{M}_{i,i} \geq \frac{1}{3}$, which means that in the limit, the probability of the walker going back to where she started is at least $\frac{1}{3}$;

(ii) [Corollary 6.5.4] There is no constant α such that $\widehat{M} = \alpha J$. If such α exists, it means that in the limit, the walker has equal chance of being on any edge, no matter which edge is the walker's initial state.

One other behavior we have looked at is periodicity. In Theorem 6.5.5, we show that for a non-trivial t-(v, k, λ_t) design with $t \geq 2$, there are no periodic states in the bipartite walk defined over it.

Generalized quadrangles are one class of t-designs with $t = 1$. A generalized quadrangle $GQ(s, t)$ is a 1-(v, k, λ) design with $k = s + 1, r = t + 1$. A coherent algebra is matrix algebra over $\mathbb{C}$ that is Schur-closed, closed under transpose and complex conjugation, and contains I and J. This is an important tool we employ to study the behavior of the bipartite walk on $GQ(s, t)$. Every coherent algebra has a unique basis of 01-matrices that are mutually orthogonal with respect to Schur multiplication. Let P, Q be orthogonal projections from the bipartite walk on $GQ(s, t)$. We show that $\langle P, Q\rangle$ is a coherent algebra. We find the unique mutually Schur-orthogonal 01-matrix basis and each matrix in the basis corresponds to a relation between flags. For example, if $(M_2)_{i,j} = 1$, it means that flags f_i, f_j share the same block.

1.2.12 Theorem (6.8.1)**.** *Let P, Q be orthogonal projections that come from the bipartite walk over the incidence graph of $GQ(s, t)$. Then $\langle P, Q\rangle$ is a homogeneous coherent algebra and*

$$\{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}$$

is the unique mutually orthogonal (with respect to Schur multiplication) basis of $\langle P, Q\rangle$ that consists of 01*-matrices.* □

We show that

$$U, H, A(\overrightarrow{H}), A(H), \widehat{M_U} \in \langle P, Q\rangle.$$

This enables us to write each of $\{U, H, A(\overrightarrow{H}), A(H), \widehat{M_U}\}$ as a linear combination of M_i for $i \in \{1, \cdots, 8\}$. Using this, we get some information about the behavior of the walk.

1.2.13 Theorem (6.10.3,6.10.4)**.** *In the bipartite walk obtained from the incidence graph of a generalized quadrangle, there are no pairs of strongly cospectral flag states and no periodic states*

Chapter 2

Bipartite walks and their Hamiltonians

In this chapter, we give detailed instructions about how to construct the bipartite walk on a bipartite graph. We define the Hamiltonian of a bipartite walk and the corresponding H-(di)graph. These will be the main interest of this thesis. Using the Hamiltonian of a bipartite walk, we can draw a connection between the bipartite walk and a continuous walk. Section 3.3 will be an example of how we use this connection to construct a rare phenomenon in continuous quantum walks.

The existence of a valid H-digraph will be crucial for us to draw the connection. Given the bipartite walk defined on G, it is not obvious how the structure of G affects the walk. But we are able to show there exists a valid H-digraph if and only if the adjacency matrix of G is invertible. When G is biregular, we show that the spectrum of the line graph of G determines the spectrum of the transition matrix U of the walk. Later in Section 5.3, we are able to show that G is biregular, we show that the spectrum of U is determined by the spectrum of $A(G)$. From this, we draw a correspondence between the spectrum of G and that of its line graph for a biregular G.

Spectral analysis will be the main approach used in this thesis. We present a complete characterization by Zhan in [37] on the eigenvalues and eigenspaces of the transition matrix of a bipartite walk.

The results in the first three sections of this chapter can also be found in my paper with Godsil, Sobchuk and Zhan [9].

2.1 Bipartite walks

All the notation introduced in this section will be followed throughout the thesis unless explicitly stated otherwise.

Let G be a bipartite graph with two parts C_0, C_1. Now we define two partitions of the edges of G, denoted by π_0, π_1 respectively. If two edges have the same end x in C_0, then they belong to the same cell of π_0. Similarly, if two edges have the same end y in C_1, then they belong to the same cell of π_1.

Given a matrix M, we *normalize* it by scaling each column of ρ to a unit vector and the resulting matrix is called the normalized M. Let P_0, P_1 be the characteristic matrices of π_0, π_1 respectively. That is, for $i \in \{0, 1\}$, the rows of P_i are indexed by edges of G and the columns are indexed by vertices in C_i and

$$(P_i)_{s,t} = \begin{cases} 1, & \text{if vertex } t \text{ is an end of edge } s; \\ 0, & \text{otherwise.} \end{cases}$$

Let $\widehat{P}_0, \widehat{P}_1$ denote the normalized P_0, P_1 and define

$$P = \widehat{P}_0 \widehat{P}_0^T, \quad Q = \widehat{P}_1 \widehat{P}_1^T.$$

Then P, Q are the projections, i.e.,

$$P^2 = P, \quad Q^2 = Q.$$

We can see that P, Q are projections onto the vectors that are constant on the cells of π_0, π_1 respectively.

Reflections are orthogonal mappings. Given a subspace W of of a vector space V, a *reflection* in W is the linear mapping that fixes every element in W and act as $-I$ on $W^\perp$. Since P is a projection, we have that

$$(2P - I)^2 = 4P^2 - 4P + I = I,$$

which implies that $2P - I$ is unitary with order two. For every vector $v \in \operatorname{im}(P)$ and $u \in \ker(P)$,

$$(2P - I)v = v, \quad (2P - I)u = -u.$$

Thus, we can see that $2P - I$ is the reflection in $\operatorname{im}(P)$. Similarly, we can argue that $2Q - I$ is the reflection in $\operatorname{im}(Q)$.

The transition matrix of the bipartite walk defined on G is

$$U = \left(2\widehat{P}_0\widehat{P}_0^T - I\right)\left(2\widehat{P}_1\widehat{P}_1^T - I\right) = (2P - I)\,(2Q - I)\,.$$

Rows and columns of U are indexed by edges of G. The state space are complex functions on edges of G. We identify edges of G with standard basis vectors $e_1, e_2, \cdots, e_{|E(G)|}$. Given initial state e_a, at the k-th step, our walk is at the state

$$U^k e_a.$$

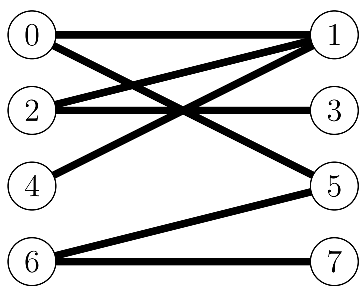


Figure 2.1: Bipartite graph on 8 vertices

Now consider the bipartite graph G in Figure 2.1 as an example. We define the bipartite walk on G. The two parts of G are $C_0 = \{0, 2, 4, 6\}$ and $C_2 = \{1, 3, 5, 7\}$. Here is an example of how we partition edges of G: edges $\{0, 1\}, \{0, 5\}$ are in the same cell in parition π_0 and edges $\{0, 1\}, \{2, 1\}, \{4, 1\}$ are in the same cell in partition π_1. We have that

$$\widehat{P}_0 = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & 0 & \frac{1}{\sqrt{2}} \end{pmatrix}, \quad \widehat{P}_1 = \begin{pmatrix} \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

and we get the corresponding projections

$$P = \begin{pmatrix} \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & \frac{1}{2} & 0 & 0 & 0 & \frac{1}{2} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \quad Q = \begin{pmatrix} \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & 0 & \frac{1}{2} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}.$$

The transition matrix of the bipartite walk on G is

$$U = \begin{pmatrix} 0 & -\frac{1}{3} & 0 & \frac{2}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{2}{3} & 0 & \frac{2}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{2}{3} & 0 & -\frac{1}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

Let C denote the characteristic matrix of the incidence relation between π_0, π_1. That is, the rows of C are indexed by the cells of π_1 and the columns are indexed by the cells of π_0 and

$$C_{i,j} = 1$$

if there is an edge that belongs to both cell c_i in π_1 and cell c_j in π_0. In other words,

$$C = P_1^T P_0$$

and we define

$$\widehat{C} = \widehat{P}_1^T \widehat{P}_0.$$

The matrix C and $\widehat{C}$ of the bipartite graph in Figure 2.1 are

$$C = \begin{pmatrix} 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix}, \quad \widehat{C} = \begin{pmatrix} \frac{1}{\sqrt{6}} & 0 & \frac{1}{2} & 0 \\ \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{2}} & 0 & 0 \\ \frac{1}{\sqrt{3}} & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{2} & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

2.2 Spectrum of U

Spectral properties of the transition matrix U are the main machinery that we are going to use to analyze the Hamiltonian of U and the behavior of the walk. In this section, we present a complete characterization of the eigenvalues and eigenspaces of U. All the lemmas and theorems presented in this section are proved in [37] by Zhan in detail, so here we omit the proofs.

The transition matrix of a bipartite walk is of the form

$$U = (2P - I)(2Q - I)$$

and it follows that U lies in $\langle P, Q\rangle$. So, we can use the following lemma to diagonalize U.

2.2.1 Lemma (Lemma 2.3.1 in [37]). *Let P and Q be two projections acting on $\mathbb{C}^m$. Then $\mathbb{C}^m$ is a direct sum of 1- and 2-dimensional $\langle P, Q\rangle$-invariant subspaces.* □

Note the lemma above sometimes is referred to as Jordan's lemma.

Using Lemma 2.2.1, we can decompose $\mathbb{C}^m$ into a direct sum of 1- and 2-dimensional $\langle P, Q\rangle$-invariant subspaces. Then we diagonalize U restricted to each of them. The 1-dimensional $\langle P, Q\rangle$-invariant subspaces are the 1- and (-1)-eigenspace of U. They are common eigenspaces for both P and Q.

2.2.2 Theorem (Lemma 2.3.5 in [37]). *Let P, Q be projections on $\mathbb{C}^m$. The 1-eigenspace of U is*

$$(\mathrm{Col}(P) \cap \mathrm{Col}(Q)) \oplus (\ker(P) \cap \ker(Q))$$

and it has dimension

$$m - \operatorname{rk}(P) - \operatorname{rk}(Q) + 2\dim\left(\operatorname{Col}(P) \cap \operatorname{Col}(Q)\right) \qquad \square$$

Since a cell of π_0 and a cell of π_1 can intersect at most one edge, we have that

$$\operatorname{Col}(P) \cap \operatorname{Col}(Q) = \operatorname{span}\{\mathbf{1}\},$$

where $\mathbf{1}$ is the all-one vector.

2.2.3 Theorem (Lemma 2.3.6 in [37])**.** *The* (-1)*-eigenspace for* U *is*

$$(\operatorname{Col}(P) \cap \ker(Q)) \oplus (\ker(P) \cap \operatorname{Col}(Q))$$

and its dimension is

$$|C_0| + |C_1| - 2\operatorname{rk}(C). \qquad \square$$

Now we consider the complex eigenvalues of U. The following theorem is also known as the Poincaré separation theorem, or the Cauchy interlacing theorem, which is a standard result on eigenvalue interlacing.

2.2.4 Theorem (Corollary 4.3.27 in [24])**.** *Let* A *be a Hermitian matrix of size* n*. Suppose that* $1 \le m \le n$ *and let* $u_1, \cdots, u_m \in \mathbb{C}^n$ *be orthonormal. Let* $B_m = [u_i^* A u_j]_{i,j=1}$ *and let* $\lambda_1(A) \le \cdots \le \lambda_n(A)$ *and* $\lambda_1(B_m) \le \cdots \le \lambda_m(B_m)$*. Then*

$$\lambda_i(A) \le \lambda_i(B_m) \le \lambda_{i+n-m}(A), \quad i = 1, \cdots, m. \qquad \square$$

Since $\widehat{P}_1^T \widehat{P}_1 = I$, i.e., columns of $\widehat{P}_1$ are orthonormal, using the theorem above, the eigenvalues of $\widehat{C}\widehat{C}^T$ interlace those of P. In particular, we have that

$$\operatorname{Spec}\left(\widehat{C}\widehat{C}^T\right) \in [0, 1].$$

2.2.5 Lemma (Lemma 2.3.4 in [37])**.** *Let* P *and* Q *be projections on* $\mathbb{C}^m$*. Let*

$$U = (2P - I)(2Q - I).$$

Suppose $Q = LL^*$ *for some* L *with orthonormal columns. The eigenvalues of* L^*PL *lie in* $[0, 1]$*. Let* y *be an eigenvector for* L^*PL*. Let* $z = Ly$*. We have the following correspondence between eigenvectors for* L^*PL *and eigenvectors for* U*.*

(i) If y is an eigenvector for L^*PL with eigenvalue 1*, then*

$$z \in \mathrm{Col}(P) \cap \mathrm{Col}(Q).$$

(ii) If y is an eigenvector for L^*PL with eigenvalue 0*, then*

$$z \in \ker(P) \cap \mathrm{Col}(Q).$$

(iii) y is an eigenvector for L^*PL with eigenvalue $\mu \in (0,1)$, and $\theta \in \mathbb{R}$ satisfies that $2\mu - 1 = \cos(\theta)$, then

$$(\cos(\theta) + 1)\, z - \left(e^{i\theta} + 1\right) Pz$$

is an eigenvector for U with eigenvalue $e^{i\theta}$, and

$$(\cos(\theta) + 1)\, z - \left(e^{-i\theta} + 1\right) Pz$$

is an eigenvector for U with eigenvalue $e^{-i\theta}$. □

Note that in our setting, $Q = \widehat{P}_1 \widehat{P}_1^T$ and $\widehat{P}_1$ has orthonormal columns. For the purpose of this thesis, we apply the lemma above to get the eigenmatrices of U whose corresponding eigenvalues are complex.

2.2.6 Corollary (Corollary 5.2.5 in [37])**.** *Let $\mu \in (0,1)$ be an eigenvalue of $\widehat{C}\widehat{C}^T$. Choose θ such that $\cos\theta = 2\mu - 1$. Let E_μ be the orthogonal projection onto the μ-eigenspace of $\widehat{C}\widehat{C}^T$. Set*

$$W := \widehat{P}_1 E_\mu \widehat{P}_1^T.$$

Then the $e^{i\theta}$-eigenmatrix of U is

$$\frac{1}{\sin^2(\theta)} \left((\cos\theta + 1)W - (e^{i\theta} + 1)PW - (e^{-i\theta} + 1)WP + 2PWP\right),$$

and the $e^{-i\theta}$-eigenmatrix of U is

$$\frac{1}{\sin^2(\theta)} \left((\cos\theta + 1)W - (e^{-i\theta} + 1)PW - (e^{i\theta} + 1)WP + 2PWP\right). \quad \square$$

2.3 Hamiltonian

In this section, we define the Hamiltonian of a bipartite walk and the H-(di)graph associated with it. We show how the Hamiltonian help us to build a bridge between two classes of quantum walks: discrete walks and continuous walks.

For every unitary matrix U, there exist Hermitian matrices H such that

$$U = \exp(iH).$$

We call such H a *Hamiltonian* of U. Since U is unitary, it has spectral decomposition

$$U = \sum_r e^{i\theta_r} E_r = \exp(iH),$$

and we can write

$$H = -i \sum_r \log(e^{i\theta_r}) E_r = \sum_r \theta_r E_r.$$

For each eigenvalue $e^{i\theta_r}$ of U, we have that

$$\log(e^{i\theta_r}) = \log(e^{i\theta_r + 2k_r\pi})$$

for non-zero integer k_r and so, the choice of H is not unique. That is, the Hamiltonian of U is

$$H = \sum_{\theta_r} (\theta_r + 2k_r\pi) E_r,$$

for any non-zero integer k_r. Note that k_r are not necessarily equal for all the θ_r. For each eigenvalue $e^{i\theta_r}$ of U, if $k_r = 0$ and

$$-\pi < \theta_r \leq \pi,$$

the resulting unique Hamiltonian is called *the principal Hamiltonian.* Following convention, unless explicitly stated otherwise, we refer to the principal Hamiltonian to be *the Hamiltonian of* U.

Let $\overrightarrow{A}$ denote the *(weighted) skew-adjacency matrix* of a weighted oriented graph. Matrix $\overrightarrow{A}$ satisfies that if $w(i,j)$ is the weight between vertices i, j, then

$$\left(\overrightarrow{A}\right)_{i,j} = \begin{cases} w(i,j), & \text{if there is an arc from } i \text{ to } j; \\ -w(i,j), & \text{if there is an arc from } j \text{ to } i; \\ 0, & \text{otherwise.} \end{cases}$$

Let S be a real skew-symmetric matrix. Then S can be viewed as the skew-adjacency matrix of a weighted oriented graph. When $H = iS$, we define the *H-digraph* to be the weighted oriented graph whose skew-adjacency matrix is S. The *H-graph* is the underlying unweighted, non-oriented graph of the H-digraph.

There is a second class of quantum walks: *continuous quantum walks.* Here the state space is the space of complex functions on the vertices of a graph G. The walk is specified by a Hermitian matrix H with rows and columns indexed by the vertices of G (for example, the adjcency matrix of G). We then define transition matrices $U(t)$ by

$$U(t) := \exp(itH), \quad (t \in \mathbb{R}).$$

It follows that a discrete walk governed by a unitary matrix U gives rise to a continuous walk specified by a Hamiltonian of U and if the continuous walk is given by matrices $U(t)$, the transition matrix for the discrete walk is $U(1)$.

Let H be the Hamiltonian of the bipartite walk defined on a graph G. If there is a real skew symmetric S such that H can be written as $H = iS$, i.e., the H-digraph exists, then the bipartite walk defined on G is the continuous walk defined on the H-digraph over integer time. Hence, we can see the Hamiltonians help us to build a connection between discrete walks and continuous walks. Later in Section 3.3, we show how bipartite walks on paths help us to construct weighted oriented complete graphs that have universal state transfer, a rare but interesting phenomenon in continuous walks.

2.4 Existence of the H-(di)graph

It is not true that for every bipartite walk, the Hamiltonian of the walk can of the form

$$H = iS$$

for some real skew-symmetric matrix S, which means that the H-digraph does not exist in this case. The existence of the H-(di)graph is the same as the existence of a skew-symmetric S such that $H = iS$.

In this section, we will show that given a bipartite walk defined on G, the existence of the H-(di)graph is determined by G. That is, the H-(di)graph exists if and only if the adjacency matrix of G is invertible.

2.4.1 Theorem. *Let U be the transition matrix of the bipartite walk on a bipartite graph G. Let H be the Hamiltonian of U and let E_{-1} be the projection onto the (-1)-eigenspace of U. Then there is a real skew-symmetric matrix S such that*

$$H = iS + \pi E_{-1}.$$

Proof. Using the spectral decomposition

$$U = \sum_r e^{i\theta_r} E_r = \exp(iH),$$

we can write

$$H = -i \sum_r \log(e^{i\theta_r}) E_r = \sum_r \theta_r E_r,$$

where $-\pi < \theta_r \leq \pi$. It follows that the 1-eigenmatrix of U is the 0-eigenmatrix of H and the (-1)-eigenmatrix of U is the π-eigenmatrix of H and the $e^{i\theta_r}$-eigenmatrix is the θ_r-eigenmatrix of H.

Recall that $\widehat{C} = \widehat{P}_1^T \widehat{P}_0$, where $\widehat{P}_0, \widehat{P}_1$ are defined as in Section 2.1. Let $\mu \in (0,1)$ be an eigenvalue of $\widehat{C}\widehat{C}^T$. Choose θ such that $\cos\theta = 2\mu - 1$. Let F_μ be the orthogonal projection onto the μ-eigenspace of $\hat{C}\hat{C}^T$. Set

$$W := \widehat{P}_1 F_\mu \widehat{P}_1^T.$$

By Corollary 2.2.6, we have that

$$\begin{aligned} H &= \sum_{\theta_r \neq \{1,-1\}} \theta_r \left(E_r - E_{-r}\right) + \pi \cdot E_{-1} \\ &= \sum_{\theta_r \neq \{1,-1\}} \theta_r \left(-\frac{2i}{\sin(\theta_r)} (PW - WP) \right) + \pi \cdot E_{-1}. \end{aligned}$$

Since $\widehat{C}\widehat{C}^T$ is real and symmetric, we know that the orthogonal projection onto its μ-eigenspace F_μ is real and symmetric. It follows that $W = \widehat{P}_1 F_\mu \widehat{P}_1^T$ is real and symmetric. So the matrix $PW - WP$ is real. Set

$$S = \sum_{\theta_r \neq \{1,-1\}} \theta_r \left(-\frac{2}{\sin(\theta_r)} (PW - WP) \right)$$

and we know that S is skew-symmetric. □

2.4.2 Corollary. *Let U be the transition matrix of the bipartite walk on a bipartite graph G with no isolated vertices. Then there exist a real skew-symmetric matrix S such that the Hamiltonian H of U is of the form $H = iS$ if and only if $A(G)$ is invertible.*

Proof. Since P, Q are real matrices, it follows from Theorem 2.2.3 that E_{-1}, the projection onto the (-1)-eigenspace of U, is a real matrix. By Theorem 2.4.1, there is a real skew-symmetric matrix S such that

$$H = iS + \pi E_{-1}.$$

So to prove this corollary, it is sufficient to prove that $E_{-1} = 0$ if and only if $A(G)$ is invertible.

Now consider the (-1)-eigenvalue of U. From Theorem 2.2.3, we know that the dimension of the (-1)-eigenspace of U is

$$|C_0| + |C_1| - 2\,\mathrm{rk}(C).$$

This implies that $E_{-1} = 0$ if and only if

$$|C_0| + |C_1| - 2\,\mathrm{rk}(C) = 0.$$

Since $\mathrm{rk}(P_0) = |C_0|$ and $\mathrm{rk}(P_1) = |C_1|$ and $C = P_1^T P_0$, we get that

$$\mathrm{rk}\, C \leq \min\{|C_0|, |C_1|\}.$$

Thus, $E_{-1} = 0$ if and only if $\mathrm{rk}(P_0) = \mathrm{rk}(P_1) = \mathrm{rk}(C)$, which is equivalent to requiring that C is invertible. Since

$$A(G) = \begin{pmatrix} \mathbf{0} & C \\ C^T & \mathbf{0} \end{pmatrix},$$

we can conclude that there is a real skew-symmetric S such that $H = iS$ if and only if $A(G)$ is invertible. □

In the case when $A(G)$ is not invertible, i.e., the (-1)-eigenspace of U is not empty, from the theorem above, there is no real skew-symmetric S such that the Hamiltonian H of U is of the form $H = iS$. In this case, we study the Hamiltonian of U^2.

2.5 Spectrum of line graphs determines spectrum of walks

In this section, we show that when G is biregular, the spectrum of U is determined by the spectrum of the line graph of G. Moreover, when G is d-regular, we can show that the 1-eigenmatrix of U is a sum of the (-2)- and the $2(d-1)$-eigenmatrix of the line graph of G. One nice consequence is that we are able to show that there is a correspondence between spectrum of $A(LG)$ and spectrum of $A(G)$ for a biregular G.

Give a graph G, its *vertex-edge incidence matrix* $B(G)$ is the 01-matrix with rows and columns indexed by the vertices and edges of G, respectively, such that the uf-entry of $B(G)$ is equal to one if and only if the vertex u is in the edge f.

2.5.1 Theorem. *Let G be a (d_0, d_1)-regular bipartite graph and let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix of the bipartite walk defined on G. Let the adjacency matrix of the line graph of G have spectral decomposition $A(LG) = \sum_s \lambda_s F_s$. Then we have*

$$\cos\theta_r = 2\Big(\frac{1}{d_0 d_1}\lambda_r^2 + \frac{4 - d_0 - d_1}{d_0 d_1}\lambda_r + \left(\frac{4 - 2d_0 - 2d_1}{d_0 d_1} + \frac{1}{2}\right)\Big).$$

Moreover, when $d_0 = d_1 = d$, we have that

$$\cos\theta_r = 2\left(\frac{1}{d^2}(\lambda_r + 2)^2 - \frac{2}{d}(\lambda_r + 2) + \frac{1}{2}\right) \tag{2.5.1}$$

and

$$E_1 = F_{-2} + F_{2(d-1)}. \tag{2.5.2}$$

Proof. Let B be the vertex-edge incidence matrix of G. Let LG denote the line graph of G. We have that

$$B^T B = 2I + A(LG) = d_0 P + d_1 Q, \tag{2.5.3}$$

which gives

$$(B^T B)^2 = d_0^2 P + d_1^2 Q + d_0 d_1 (PQ + QP) = 4I + A(LG)^2 + 4A(LG).$$

Rearranging the equation above, we have that

$$PQ+QP = \frac{1}{d_0d_1}\left(4I+A(LG)^2+4A(LG)-d_0\left(2I+A(LG)\right)-(d_1^2-d_0d_1)Q\right). \tag{2.5.4}$$

Given that

$$U = (2P-I)(2Q-I),$$

using Equation 2.5.3 and Equation 2.5.4, we can write

$$U+U^T = 4\left(\frac{1}{d_0d_1}A(LG)^2+\frac{4-d_0-d_1}{d_0d_1}A(LG)+\left(\frac{4-2d_0-2d_1}{d_0d_1}+\frac{1}{2}\right)I\right). \tag{2.5.5}$$

Given spectral decomposition $U=\sum_r e^{i\theta_r}E_r$, where $E_r = A_r+iB_r$, we can also write

$$U+U^T = \sum_r 2\cos\theta_r(E_r+\overline{E_r}) = \sum_r 2\cos\theta_r\cdot 2A_r. \tag{2.5.6}$$

Comparing Equation 2.5.5 and Equation 2.5.6, we have that

$$2\cos\theta_r = 4\Big(\frac{1}{d_0d_1}\lambda_r^2+\frac{4-d_0-d_1}{d_0d_1}\lambda_r+\left(\frac{4-2d_0-2d_1}{d_0d_1}+\frac{1}{2}\right)\Big).$$

When $\cos\theta_r = 1$, Equation 2.5.1 has two solutions

$$\lambda_r = -2, \quad \lambda_{r'} = 2(d-1).$$

The eigenmatrix E_1 of U is also the 1-eigenmatrix of U^T, so E_1 is the 1-eigenmatrix of $U+U^T$. Hence, we have that

$$E_1 = F_{-2}+F_{2(d-1)}. \qquad \square$$

Later in Section 5.3, we show that there is a way to write $\cos\theta_r$ in terms of eigenvalues of G. That is, if $A(G)=\sum_r \gamma_r K_r$, then

$$\cos\theta_r = 2\frac{\gamma_r^2}{d_0d_1}-1.$$

It is known that when G is regular, there is a correspondence between the spectrum of $A(LG)$ as shown in Lemma 5.4.2 ([18, Lemma 8.2.5]). We show that this is also true when G is biregular.

2.5.2 Theorem. *Let G be a (d_0, d_1)-regular bipartite graph. Let $A(LG) = \sum_s \lambda_s F_s$ be the spectral decomposition of the adjacency matrix of the line graph of G. Then for every eigenvalue λ_s of $A(LG)$,*

$$\pm\left(\sqrt{d_0 - \lambda_r - 2}\sqrt{d_1 - \lambda_r - 2}\right)$$

are eigenvalues of $A(G)$.

Proof. In Theorem 5.3.1, we show that if $A(G) = \sum_r \gamma_r K_r$, then

$$\cos\theta_r = 2\frac{\gamma_r^2}{d_0 d_1} - 1.$$

Comparing Equation 2.5.1 with the equation above, we have that

$$2\frac{\gamma_r^2}{d_0 d_1} - 1 = 2\Big(\frac{1}{d_0 d_1}\lambda_r^2 + \frac{4 - d_0 - d_1}{d_0 d_1}\lambda_r + \left(\frac{4 - 2d_0 - 2d_1}{d_0 d_1} + \frac{1}{2}\right)\Big).$$

This gives us

$$\gamma_r = \pm\left(\sqrt{d_0 - \lambda_r - 2}\sqrt{d_1 - \lambda_r - 2}\right). \qquad \square$$

2.6 Open questions

As stated in Section 2.3, for every unitary matrix U, there exist Hermitian matrices H such that

$$U = \exp(iH).$$

We can see the choice of H is not unique. That is, the Hamiltonian of U is

$$H = \sum_{\theta_r} (\theta_r + 2k_r\pi)E_r,$$

for any non-zero integer k_r. Out of convention, we choose the principal Hamiltonian to be the Hamiltonian with $k_r = 0$ and $-\pi < \theta_r \leq \pi$. One question we would like to post here is

1. Can we get more information about the walk by choosing different values of k_r and θ_r?

Chapter 3

Paths and Even Cycles

Two of the simplest classes of bipartite graphs are paths and even cycles. In this chapter, we show that the transition matrices of bipartite walks defined on paths and even cycles are cyclic permutations. Also, we show that there is perfect state transfer between every pair of states on bipartite walk defined on paths. This is a rare phenomenon called universal state transfer.

We are also able to show that when n is even, the H-digraph obtained from the bipartite walk on P_n is a oriented weighted K_{n-1}. Using this, we construct a infinite family of weighted oriented K_n for odd n such that the continuous walks defined on them have universal state transfer. This shows another motivation for us to study bipartite walks. Since the Hamiltonians of bipartite walks connect bipartite walks and continuous walks on its H-digraph, we can use bipartite walks to construct interesting phenomena in continuous walks.

3.1 Paths

Give a path P_n on n vertices, we label the vertices of P_n as $v_0, v_1 \cdots, v_{n-1}$ accordingly from the leftmost vertex to the rightmost vertex of P_n. Note that v_0, v_{n-1} are the only two vertices of degree 1 with all the others of degree 2.

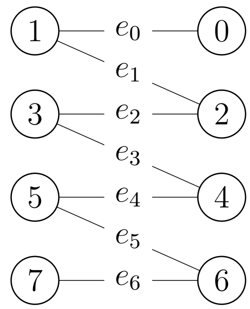


Figure 3.1: P_8

Based on the ordering of the vertices of P_n, we have that

$$C_0 = \{v_i : 0 \leq i \leq n-1 \text{ and } i \text{ is odd}\},$$
$$C_1 = \{v_i : 0 \leq i \leq n-1 \text{ and } i \text{ is even}\}.$$

Partition π_0 is the partition of edges such that edges with the same end in C_0 are in the same cell of π_0. Partition π_1 is the partition of edges such that edges with the same end in C_1 are in the same cell of π_1. We use e_i to denote the edge $\{v_i, v_{i+1}\}$ for all integer $0 \leq i \leq n-2$. So,

$$E(P_n) = \{e_0, \cdots, e_{n-2}\}.$$

Recall that P, Q are the projections onto the vectors that are constant on the cells of π_0, π_1 respectively. Let c_i denote the characteristic vector of the edges adjacent to vertex i, i.e., the j-th entry of c_i

$$c_i(j) = \begin{cases} 1 & \text{if vertex } i \text{ is one end of edge } e_j, \\ 0 & \text{otherwise.} \end{cases}$$

The matrix $2Q - I$ is a reflection about the column space of Q and the column space of Q is

$$\text{Col}(Q) = \text{span}\{c_0, c_2, \cdots, c_{n-2}\},$$

which is the span of cells of π_1. If two edges belong to the same cell, then we say they are *cellmates* of each other.

Since every vertex of a path has degree ≤ 2, every edge has at most one cellmate in each of the partitions. For each $0 \leq i \leq n-2$, let e_j be the cellmate of e_i in π_0. Note that it is possible that $i = j$. Using that each cell in π_0 has size ≤ 2, we have that

$$(2P - I)e_i = e_j.$$

Similarly, if e_i, e_j are cellmates in π_1 (i, j are not necessarily distinct), then we have that

$$(2Q - I)e_i = e_j.$$

Here both reflections $2P - I$ and $2Q - I$ are permutation matrices. Thus, the transition matrix $U = (2P - I)(2Q - I)$ of the bipartite walk on P_n is a permutation matrix.

For $0 \leq i \leq n-2$, if n is odd,

$$Ue_i = \begin{cases} e_{i+2}, & \text{if } i \text{ is odd and } i \neq n-2; \\ e_{i-2}, & \text{if } i \text{ is even and } i \neq 0; \\ e_1, & \text{if } i = 0; \\ e_{n-3}, & \text{if } i = n-2; \end{cases} \tag{3.1.1}$$

if n is even, then

$$Ue_i = \begin{cases} e_{i+2}, & \text{if } i \text{ is odd and } i \neq n-3; \\ e_{i-2}, & \text{if } i \text{ is even and } i \neq 0; \\ e_1, & \text{if } i = 0; \\ e_{n-2}, & \text{if } i = n-3. \end{cases} \tag{3.1.2}$$

3.1.1 Theorem. *The transition matrix of the bipartite walk on P_n is an $(n-1)$-cycle permutation whose cycle form is*

$$(e_0, e_1, e_3, \cdots, e_{n-4}, e_{n-2}, e_{n-3}, e_{n-5}, \cdots, e_2)$$

if n is odd, and

$$(e_0, e_1, e_3, \cdots, e_{n-5}, e_{n-3}, e_{n-2}, e_{n-4}, \cdots, e_2)$$

if n is even.

Proof. It follows from the discussion above. □

For example, the transition matrix of the bipartite walk on P_8 is

$$U(P_8) = \begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

This corresponds to the permutation (0135642) in S_7, and we have that

$$U(P_8)^7 = I.$$

Since $U(P_8)$ is a permutation matrix of order 7, it is easy to see that every edge of P_8 can be mapped to any other edges within 7 steps in the bipartite walk. This is an interesting phenomenon called *universal perfect state transfer*. Note that if U is the transition matrix of the bipartite walk on P_n, then

$$U^{n-1} = I,$$

which implies that for every n, the bipartite walk on P_n has the universal perfect state transfer. We will discuss this property further in the next section.

When n is even, the transition matrix $U(P_n)$ is a cyclic permutation matrix of order $n-1$. It has eigenvalue

$$\lambda_k = \left(e^{\frac{2\pi i}{n-1}}\right)^k$$

with eigenvector

$$f_k = \begin{pmatrix} 1 & \lambda_k^{-1} & \lambda_k & \lambda_k^{-2} & \lambda_k^2 & \cdots & \lambda_k^{-(n-2)/2} & \lambda_k^{(n-2)/2} \end{pmatrix}^T, \tag{3.1.3}$$

for $k = 0, \cdots, n-2$. The λ_k-eigenspace of U is

$$E_{\lambda_k} = \frac{1}{n-1} f f^*.$$

Note that $E_1 = \frac{1}{n-1} J$, where J is the all-one matrix.

From the eigenvectors (3.1.3) of U, when n is even, if s, t are integers in $\{1, \cdots, n-1\}$, we have that

$$(E_{\lambda_r})_{s,t} = \begin{cases} \frac{1}{n-1}(\lambda_r)^{-\frac{s}{2}}(\lambda_r)^{\frac{t}{2}} & \text{if both } s, t \text{ are even;} \\ \frac{1}{n-1}(\lambda_r)^{\frac{s-1}{2}}(\lambda_r)^{\frac{t}{2}} & \text{if } s \text{ is odd and } t \text{ is even;} \\ \frac{1}{n-1}(\lambda_r)^{-\frac{s}{2}}(\lambda_r)^{-\frac{t-1}{2}} & \text{if } s \text{ is even and } t \text{ is odd;} \\ \frac{1}{n-1}(\lambda_r)^{\frac{s-1}{2}}(\lambda_r)^{-\frac{t-1}{2}} & \text{if both } s, t \text{ are odd.} \end{cases} \tag{3.1.4}$$

3.1.2 Theorem. *For an even $n \geq 4$, the H-digraph obtained from the bipartite walk on P_n is an oriented K_{n-1}.*

Proof. As the discussion above, the transition matrix of bipartite walk on P_n has spectral decomposition

$$U = \sum_{k=0}^{n-2} \lambda_k E_{\lambda_k},$$

where

$$\lambda_k = \left(e^{\frac{2\pi i}{n-1}}\right)^k.$$

When n is even, the Hamiltonian of U is

$$H = \sum_{k=0}^{(n-2)/2} \frac{2k\pi}{n-1}\left(E_{\lambda_k} - \overline{E_{\lambda_k}}\right).$$

To show that the H-digraph is an oriented complete graph, we show that the Hamiltonian H has zero diagonal and all its off-diagonal entries are non-zero. We have shown above that the eigenvector of U with eigenvalue λ_k is of the form 3.1.3, so each row of E_{λ_k} is a permutation of its first row, which implies that each row of H is a permutation of its first row. In order to prove that all the off-diagonal entries of H are non-zero, it is sufficient to prove that

$$H_{1,t} \neq 0$$

for all $t \in \{1, 2, \cdots, n-1\}$.

Based on the formulas of the (s,t)-th entry of E_{λ_r} given in Equation 3.1.4, we have that

$$\left(E_{\lambda_r}-\overline{E_{\lambda_r}}\right)_{s,t}=\begin{cases}\frac{2}{n-1}\sin\left(\frac{2\pi r}{n-1}\cdot\frac{t-s}{2}\right)i, & \text{if both } s,t \text{ are even;}\\ \frac{2}{n-1}\sin\left(\frac{2\pi r}{n-1}\cdot\frac{s+t+1}{2}\right)i, & \text{if } s \text{ is odd and } t \text{ is even;}\\ \frac{2}{n-1}\sin\left(\frac{2\pi r}{n-1}\cdot\frac{-t-s-1}{2}\right)i, & \text{if } s \text{ is even and } t \text{ is odd;}\\ \frac{2}{n-1}\sin\left(\frac{2\pi r}{n-1}\cdot\frac{s-t}{2}\right)i, & \text{if both } s,t \text{ are odd;}\\ 0 \quad \text{if } s=t\end{cases}$$

for $r\in\{0,1,2,\cdots,n-2\}$ and, $s,t\in\{1,\cdots,n-1\}$. Then entries of the first row of H are

$$(H)_{1,t}=\sum_{k=0}^{(n-2)/2}\frac{2k\pi}{n-1}\left(E_{\lambda_k}\right)_{1,t}=\begin{cases}\sum_{k=0}^{(n-2)/2}\frac{4k\pi}{(n-1)^2}\sin\left(\frac{2k\pi}{n-1}\cdot\frac{1-t}{2}\right) & \text{if } t \text{ is odd and } t\neq 1;\\ \sum_{k=0}^{(n-2)/2}\frac{4k\pi}{(n-1)^2}\sin\left(\frac{2k\pi}{n-1}\cdot\frac{2+t}{2}\right) & \text{if } t \text{ is even;}\\ 0 \quad \text{if } t=1.\end{cases}$$

If t is odd and $t\neq 1$, we have that

$$(H)_{1,t}=\frac{\pi\csc\left(\frac{\pi(t-1)}{2(n-1)}\right)\left(n\sin\left(\frac{t\pi}{2}\right)-\sin\left(\frac{n(t-1)\pi}{2(n-1)}\right)\csc\left(\frac{(t-1)\pi}{2(n-1)}\right)\right)}{(n-1)^2} \tag{3.1.5}$$

and if t is even, we have that

$$(H)_{1,t}=\frac{\pi\csc\left(\frac{\pi(t+2)}{2(n-1)}\right)\left(n\cos\left(\frac{t\pi}{2}\right)+\sin\left(\frac{n(t+2)\pi}{2(n-1)}\right)\csc\left(\frac{(t+2)\pi}{2(n-1)}\right)\right)}{(n-1)^2}. \tag{3.1.6}$$

From Equation 3.1.5, since $-1\leq\sin(\theta)\leq 1$ for all θ and $\sin\left(\frac{t\pi}{2}\right)\in\{1,-1\}$, in order to get $(H)_{1,t}=0$, there must exist an odd integer $t\in\{3,\cdots,n-1\}$ such that

$$\csc\left(\frac{(t-1)\pi}{2(n-1)}\right)=\pm n.$$

Let $t=2l+1\in\{1,\cdots,n-1\}$. Solving

$$\csc\left(\frac{2l\pi}{2(n-1)}\right)=n,$$

we get two roots

$$l_1 = \frac{(n-1)\left(2\pi h - \sin^{-1}\left(\frac{1}{n}\right) + \pi\right)}{\pi}$$

and

$$l_2 = \frac{(n-1)\left(2\pi h + \sin^{-1}\left(\frac{1}{n}\right)\right)}{\pi}$$

for $n \neq 0$, $n \neq 1$ and $h \in \mathbb{Z}$. But there is no even $n \geq 2$ such that $l_1 \in \mathbb{Z}$ or $l_2 \in \mathbb{Z}$. Similarly,

$$\csc\left(\frac{2l\pi}{2(n-1)}\right) = -n,$$

has roots

$$l_3 = \frac{(n-1)\left(2\pi h + \sin^{-1}\left(\frac{1}{n}\right) + \pi\right)}{\pi}$$

and

$$l_4 = \frac{(n-1)\left(2\pi h - \sin^{-1}\left(\frac{1}{n}\right)\right)}{\pi}$$

for $n \neq 0$, $n \neq 1$ and $h \in \mathbb{Z}$. There is also no even $n \geq 2$ such that $l_3 \in \mathbb{Z}$ or $l_4 \in \mathbb{Z}$.

Similarly, based on Equation 3.1.6, since $\sin(x) \in [-1, 1]$ and $\cos\left(\frac{t\pi}{2}\right) \in \{1, -1\}$, for the $(1, t)$-entry of H to be zero, there must exist an even integer $t \in \{1, \cdots, n-1\}$ such that

$$\csc\left(\frac{(t+2)\pi}{2(n-1)}\right) = \pm n.$$

Let $t = 2x + 2 \in \{1, \cdots, n-1\}$. Solving

$$\csc\left(\frac{(2x+4)\pi}{2(n-1)}\right) = n,$$

we get two roots

$$x_1 = 2hn - 2h + n - \frac{(n-1)\sin^{-1}\left(\frac{1}{n}\right)}{\pi} - 3$$

and

$$x_2 = 2h(n-1) + \frac{(n-1)\sin^{-1}\left(\frac{1}{n}\right)}{\pi} - 2$$

for $n \neq 0$, $n \neq 1$ and $h \in \mathbb{Z}$. Equation

$$\csc\left(\frac{(2x+4)\pi}{2(n-1)}\right) = -n$$

has roots

$$x_3 = 2hn - 2h + n + \frac{(n-1)\sin^{-1}\left(\frac{1}{n}\right)}{\pi} - 3$$

and

$$x_4 = 2h(n-1) - \frac{(n-1)\sin^{-1}\left(\frac{1}{n}\right)}{\pi} - 2$$

for $n \neq 0$, $n \neq 1$ and $h \in \mathbb{Z}$. There is no even $n \geq 2$ such that any one of x_1, x_2, x_3, x_4 can be an integer.

So we can conclude that

$$(H)_{1,t} \neq 0$$

for all $t \in \{2, \cdots, n-1\}$. From Equation 3.1.4, it is easy to see that H had zero diagonal.

Therefore, the H-digraph is an oriented K_{n-1}. $\square$

When n is odd, the adjacency matrix of P_n is not invertible. By Corollary 2.4.2, there does not exist an H-(di)graph. So instead, when n is odd, we consider the H-(di)graph of $U(P_n)^2$. When $n = 3$, the Hamiltonian of U^2 is zero matrix. When $n \equiv 1 \pmod 4$, the square of its transition matrix $U(P_n)^2$ still has -1 as an eigenvalue, which implies that there is no real skew-symmetric S such that Hamiltonian of $U(P_n)^2$ is of the form iS. Even though it is possible that we can get rid of the (-1)-eigenmatrix of $U(P_n)$ by repeatedly taking U to the power of two , it will not provide any more insight on either the Hamiltonian or the corresponding H-(di)graph. So here, we omit the case when $n \equiv 1 \pmod 4$.

3.1.3 Corollary. *When $n \equiv 3 \pmod 4$, let H be the Hamiltonian of $U(P_n)^2$, then H-digraph is two copies of weighted oriented $K_{\frac{n-1}{2}}$.*

Proof. By Theorem 3.1.1, when n is odd, the matrix $U(P_n)^2$ corresponds to two $\left(\frac{n-1}{2}\right)$-cycle permutations in $S_{\frac{n-1}{2}}$. It follows that the H-(di)graph is two copies of the H-(di)graph of $U(P_{\frac{n+1}{2}})$. The result follows from Theorem 3.1.2. $\square$

3.2 Even cycles

Another class of simple bipartite graphs is even cycles. We study bipartite walks defined on even cycles using the same approach shown in previous section.

For an even integer n, given a path P_n with the same vertex labeling as described in previous section, we add an edge e_{n-1} between v_0, v_{n-1}, which gives us a even cycle C_n. Define two parts of $V(C_n)$ as

$$C_0 = \{v_i : 0 \leq i \leq n-1 \text{ and } i \text{ is odd}\},$$
$$C_1 = \{v_i : 0 \leq i \leq n-1 \text{ and } i \text{ is even}\}.$$

If two edges share a same end in C_0, then they are in the same cell of partition π_0. If two edges share a same end in C_1, then they are in the same cell of partition π_1.

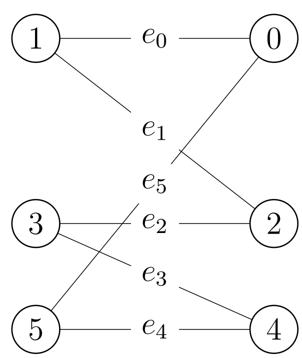


Figure 3.2: C_6

When n is even, let $U(C_n)$ be the transition matrix of the bipartite walk on C_n. Since every cell of π_0, π_1 contains exactly two edges, using the same argument as the one in previous section, we have that $U(C_n)$ is a permutation matrix. In particular, we have that

$$U(C_n)e_i = \begin{cases} e_{i+2 \pmod n} & \text{if } i \text{ is odd;} \\ e_{i-2 \pmod n} & \text{if } i \text{ is even.} \end{cases} \tag{3.2.1}$$

3.2.1 Theorem. *When n is even, the transition matrix of the bipartite walk on C_n is a cyclic permutation matrix of order $n/2$. It has cycle form*

$$(e_0, e_{n-2}, \cdots, e_2)(e_1, e_3, \cdots, e_{n-1}).$$

Proof. If follows directly from the mapping relation 3.2.1. □

Note that the eigenvalues of C_n are

$$\left\{ 2\cos\left(\frac{2\pi k}{n}\right) : k \in \{0, 1, \cdots, n-1\} \right\}.$$

So when $n \equiv 0 \pmod 4$, the adjacency matrix of C_n is not invertible and we consider the Hamiltonian of $U(C_n)^2$ instead.

3.2.2 Corollary. *Let $U(C_n)$ be the transition matrix of bipartite walk on C_n for some even n. When $n \equiv 2 \pmod 4$, let H be the Hamiltonian of $U(C_n)$, then the corresponding H-digraph is two copies of a weighted oriented $K_{\frac{n}{2}}$. When $n \equiv 0 \pmod 4$ and $n \geq 12$, let H be the Hamiltonian of U^2, then the corresponding H-digraph is four copies of a weighted oriented $K_{\frac{n}{4}}$.*

Proof. From Theorem 3.2.1, the transition matrix of U is two $\frac{n}{2}$-cycles and each cycle is the permutation associated with the transition matrix of bipartite walk on $P_{\frac{n}{2}+1}$. Results follow from Theorem 3.1.2 and Corollary 3.1.3. □

Note that when $n = 4$, the Hamiltonian of $U(C_n)$ is zero matrix. When $n = 8$, the transition matrix $U(C_n)$ and $U(C_n)^2$ both have -1 as eigenvalues. There is no real skew-symmetric S such that the Hamiltonian of $U(C_n)$ or the Hamiltonian of $U(C_n)^2$ is of the form iS and so, we omit the case when $n = 8$.

3.3 Universal perfect state transfer

Let U be the transition matrix of the continuous walk defined over the graph G and let the standard basis e_a represent the state a. Then we say there is *perfect state transfer* from state a to state b if

$$|U(t)_{a,b}|^2 = 1.$$

A graph G has *universal perfect state transfer* if it has perfect state transfer between every pair of its vertices. According to Cameron et al. in [6], the only known graphs that have universal perfect state transfer are oriented K_2, C_3 with constant weight i assigned on each arc.

In this section, we show that bipartite walk can help us construct weighted oriented graphs where the continuous quantum walk has universal perfect state transfer. Note that when we talk about continuous walks on weighted oriented graphs, the Hamiltonian is the weighted skew-adjacency matrix $\overrightarrow{A}$ of the graph. The transition matrix of the walk defined on the weighted oriented graph is

$$\exp(i\overrightarrow{A}).$$

One easy observation is that if the transition matrix U of a bipartite walk is a permutation matrix with finite order and the corresponding permutation has exactly one orbit, then the continuous walk defined on its H-digraph has universal perfect state transfer.

We have shown in Theorem 3.1.1 that when n is even, the transition matrix of the bipartite walk over P_n is a permutation matrix with order $n-1$. We can use this to construct weighted graphs over which continuous walks have universal perfect state transfer.

The following corollary shows us how to construct a weighted oriented complete graph such that the continuous walk defined on it has universal perfect state transfer.

3.3.1 Corollary. *Let n be an even integer. Let s, t be distinct integers in $\{1, \cdots, n-1\}$. We define*

$$\alpha = \begin{cases} \frac{t-s}{2}, & \textit{if both } s,t \textit{ are even;} \\ \frac{s+t+1}{2} & \textit{if } s \textit{ is odd and } t \textit{ is even;} \\ \frac{-t-s-1}{2}, & \textit{if } s \textit{ is even and } t \textit{ is odd;} \\ \frac{s-t}{2}, & \textit{if both } s,t \textit{ are odd.} \end{cases}$$

Let

$$w(s,t) = \frac{2}{n-1} \sum_{r=1}^{\frac{n}{2}-1} \frac{2\pi r}{(n-1)} \sin\left(\frac{2\pi r}{n-1}\alpha\right).$$

If $w(s,t) > 0$, we orient the edge $\{s,t\}$ from s to t and give it weight $w(s,t)$ and if $w(s,t) < 0$, we orient the edge $\{s,t\}$ from t to s and give it weight $-w(s,t)$ for all distinct $s,t \in \{1, \cdots, n-1\}$. If $w(s,t) = 0$, there is no arc between s and t. Let $\overrightarrow{A}$ be the weighted skew-adjacency matrix of the resulting weighted oriented K_{n-1}. Then the continuous walk with transition matrix $\exp\left(i\overrightarrow{A}\right)$ has universal perfect state transfer and every state will get transferred perfectly to any other state within time $t \leq n-1$.

Proof. The corollary follows directly from Theorem 3.1.1 and Theorem 3.1.2. □

The construction described in the corollary above give us an infinite family of weighted oriented graphs with universal perfect state transfer.

Consider the bipartite walk defined on P_8. The Hamiltonian H of $U(P_8)$ can be written as $H = iS$ where S is a skew-symmetric matrix. Due to the limited space we have, we round S to the nearest hundredth and

$$S \approx \begin{pmatrix} 0.0 & 1.03 & -1.03 & -0.57 & 0.57 & 0.46 & -0.46 \\ -1.03 & 0.0 & 0.57 & 1.03 & -0.46 & -0.57 & 0.46 \\ 1.03 & -0.57 & 0.0 & 0.46 & -1.03 & -0.46 & 0.57 \\ 0.57 & -1.03 & -0.46 & 0.0 & 0.46 & 1.03 & -0.57 \\ -0.57 & 0.46 & 1.03 & -0.46 & 0.0 & 0.57 & -1.03 \\ -0.46 & 0.57 & 0.46 & -1.03 & -0.57 & 0.0 & 1.03 \\ 0.46 & -0.46 & -0.57 & 0.57 & 1.03 & -1.03 & 0.0 \end{pmatrix}$$

For each edge (s,t) of K_7, we assign it with the weight of the value of the (s,t)-entry of S. To show an example, we assign some edges in K_7 in Figure 3.3. The continuous walk defined on the resulting graph has universal perfect state transfer and for any state a, b, there is perfect state transfer from state a to state b within time $t \leq 7$.

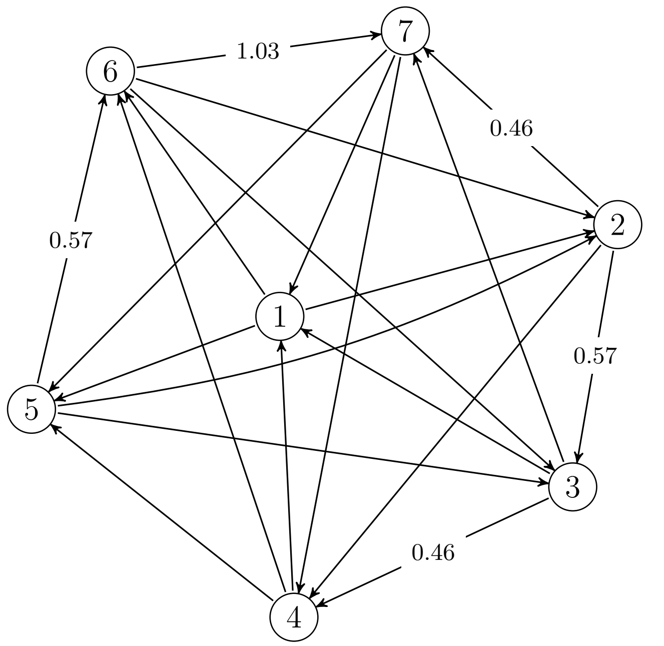


Figure 3.3: the weighted K_7 obtained from bipartite walk on P_8

3.4 Open questions

One feature that distinguishes continuous quantum walks and discrete quantum walks is that perfect state transfer does not have to be symmetric in discrete walks. In a continuous walk, since the Hamiltonian is symmetric, perfect state transfer is symmetric, i.e., there exists a time t such that there is perfect state transfer from state a to state b and from state b to a. However, in general, the transition matrix of a discrete quantum walk is not symmetric. Consequently, perfect state transfer in discrete walks is not necessarily symmetric.

Recall that the transition matrix of the bipartite walk defined on the graph in Figure 2.1 is

$$U = \begin{pmatrix} 0 & -\frac{1}{3} & 0 & \frac{2}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & \frac{2}{3} & 0 & \frac{2}{3} & \frac{1}{3} & 0 & 0 \\ 0 & \frac{2}{3} & 0 & -\frac{1}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}.$$

It is easy to see that there is perfect state transfer from state e_1 to e_6 at step $k = 1$. But up to $k = 300000$ steps, there is no perfect state transfer observed from e_6 to e_1. We suspect that there is no perfect state transfer from e_6 to e_1.

In bipartite walks, perfect state transfer does not have to be symmetric. We would like to find a condition on graph G that determines whether or not perfect state transfer is symmetric.

Among all the bipartite walks we have observed, if the walk has perfect state transfer, then the underlying graph has minimum degree at most two. We would like to know if there is any graph G with minimum degree at least three that has perfect state transfer in the bipartite walk.

So far, all the bipartite walks we have observed that have universal perfect state transfer come from paths. In other words, their transition matrices are permutation matrices. So, we would like to know that if there is a walk whose transition matrix is not a permutation matrix that has universal perfect state transfer.

Chapter 4

Grover's Walks

Grover's walk is a well-studied discrete quantum walk model. It can be used to implement Grover's search algorithm, which is one of the most important application of quantum walks.

Given a graph G, let $U_{\mathrm{GW}}(G)$ be the transition matrix of Grover's walk on G and let $U_{\mathrm{BW}}(S(G))$ be the transition matrix of the bipartite walk on the subdivision graph of G. We are going to show that Grover's walk is a special case of bipartite walk model. That is,

$$U_{\mathrm{GW}}(G) = U_{\mathrm{BW}}(S(G)).$$

Moreover, we can show that if G is a bipartite graph,

$$U_{GW}(G)^{2k} = \begin{pmatrix} (U_{BW}(G))^k & 0 \\ 0 & \left(U_{BW}^T(G)\right)^k \end{pmatrix}$$

for any positive integer k.

4.1 Grover's iteration

Given an unstructured database containing n elements, there is only one element that is "marked" and our goal is to find the marked element. Any classical algorithm will take $\mathcal{O}(n)$ steps to find the target. In [22], Grover proposes a quantum algorithm that only needs $\mathcal{O}(\sqrt{n})$ to identify the marked element.

We are going to describe the Grover's iteration used in Grover's search algorithm. A full description of Grover's search algorithm can be found in [19, Chapter 6].

We identify the n elements in the database using the standard basis vectors $e_1, e_2, \cdots, e_n$ of the complex inner product space $\mathbb{C}^n$. Assume that e_j is the marked element. Recall that if W is a subspace of a vector space V, a reflection in W is the linear mapping that fixes each element in W and acts as $-I$ on $W^\perp$. Let τ_j be a reflection on $e_j^\perp$, i.e.,

$$\tau_j(x) = x - 2\frac{\langle e_j, x\rangle}{\langle e_j, e_j\rangle} e_j$$

and the matrix representation of τ_j is

$$V_j = 2E_{j,j} - I,$$

where $E_{j,j}$ is the matrix with 1 in its (j,j)-entry and 0 otherwise. It is easy to check that V_j is unitary. Operator τ_j is the oracle query used in Grover's search algorithm. We use τ_j to mark the target element. Similarly, let $\mathbf{1}$ be the all-one vector and define

$$x_0 = \frac{1}{\sqrt{n}}\mathbf{1}$$

and we define τ_0 be a reflection on $x_0^\perp$. Let J denote the all-one matrix and

$$V_0 = \frac{2}{n}J - I$$

is the matrix representation of the map τ_0, which is unitary. Matrix V_0V_j is the *Grover's iteration*, which is also unitary. It is the operator used in Grover's search algorithm.

For Grover's search algorithm, the initial state is set to be x_0 and the system evolves according to V_0V_j. At the k-th step, the system will be in the state

$$\left(V_0V_j\right)^k x_0.$$

Then we measure the system at k-th step relative to the standard basis, which means that at k-th step, the system is in the state e_j with probability

$$\left|\langle \left(V_0V_j\right)^k x_0, e_j\rangle\right|^2.$$

Grover's algorithm says that there exists a $k \in \mathcal{O}(\sqrt{n})$ such that after k iterations, the system is in the state e_j with high probability. Comparing to its classical analogue, Grover's algorithm provides a quadratic speedup.

4.2 Grover's search using quantum walks on graphs

Now we will show that how we can define a quantum walk on the complete graph K_n with one loop on each of its vertices to implement Grover's algorithm. This implementation was first described by Ambainis, Kempe and Rivosh [3]. The description provided below is due to Godsil, Zhan [20, Section 1.5,1.6].

Consider the system with state space $\mathbb{C}^n \otimes \mathbb{C}^n$. We can view $\mathbb{C}^n$ as the space of complex functions on the vertices of the complete graph K_n. Along the same lines, we can view $\mathbb{C}^n \times \mathbb{C}^n$ as the space of complex functions on arcs and loops of K_n with one loop on each of its vertices. In this case, vector $e_u \otimes e_u$ corresponds to a loop on vertex u.

Define a permutation operator R such that

$$R(e_i \otimes e_j) = e_j \otimes e_i.$$

Note that

$$R(\tau_j \otimes \tau_0)R = \tau_0 \otimes \tau_j.$$

We have that

$$\left(R(\tau_j \otimes \tau_0)\right)^{2k} = (\tau_0\tau_j)^k \otimes (\tau_j\tau_0)^k.$$

It follows that the action of

$$U := R(\tau_j \otimes \tau_0)$$

is determined by the action of $\tau_0\tau_j$ and $\tau_j\tau_0$ on $\mathbb{C}^n$. Since τ_0, τ_j are reflections, we have that $\tau_j\tau_0 = (\tau_0\tau_j)^{-1}$. Since $\tau_0\tau_j$ is the operator used in Grover's algorithm, we can define a quantum walk on arcs and loops of K_n to implement Grover's search algorithm.

If the initial state is

$$x_0 \otimes x_0 = \frac{1}{n}\mathbf{1} \otimes \mathbf{1},$$

then

$$U^{2k}(x_0 \otimes x_0) \approx e_j \otimes \left((\tau_j\tau_0)^k x_0\right).$$

So at step $2k$, we measure the first register yields e_j with high probability.

Let G be the complete graph on n vertices with one loop on each of its vertices. If vertices u and v are adjacent, we write $u \sim v$. An *arc* is an ordered pair of adjacent vertices. Let $\alpha = (x, y)$ be an arc. We say x is the *head* of α, denoted by $o(\alpha)$ and y is the *tail* of α, denoted by $t(\alpha)$. As we described before, the characteristic vector of the arc (u, v) is $e_u \otimes e_v$. The state space $\mathbb{C}^n \otimes \mathbb{C}^n$ is spanned by the characteristic vectors of arcs of G. Then the initial state of Grover's algorithm is

$$x_0 \otimes x_0 = \frac{1}{n} \sum_{u \sim v} e_u \otimes e_v,$$

a constant function that maps each arc to $\frac{1}{n}$. Operator $\tau_j \otimes \tau_0$ is the *coin operator* and the matrix representation of it is

$$V_j \otimes V_0 = \left(2 e_j e_j^T - I\right) \otimes \left(\frac{2}{n} J - I\right).$$

We apply coin operator to arc (u, v) and we get that

$$(\tau_j \otimes \tau_0)(e_u \otimes e_v) = \begin{cases} e_u \otimes \left(\frac{1}{\sqrt{n}} \sum_{w \sim u} e_w\right), & \text{if } u \neq j; \\ e_u \otimes \left(-\frac{1}{\sqrt{n}} \sum_{w \sim u} e_w\right), & \text{if } u = j. \end{cases}$$

We can see that applying the coin operator, the quantum walker redistribute her amplitudes over the outgoing arcs of current tail u.

We can write

$$U = R(V_j \otimes V_0) = R\left(I \otimes V_0\right)\left(V_j \otimes I\right)$$

and define

$$U_0 = R\left(I \otimes V_0\right), \quad U_1 = V_j \otimes I.$$

We can see that U_0 defines a quantum walk on G and its coin operator $I \otimes V_0$ treats all the vertices equally. But the action of U_j on the marked vertex is different from its action on unmarked vertices. In particular, it acts as $-I$ on outgoing arcs of j and it acts as I on all the other arcs.

4.3 Grover's walks

The main interest of this thesis will be quantum walks on graphs with no marked vertex, which is a generalization of the walk defined by U_0. Given a graph G, we assign *the Grover coin*

$$\frac{2}{\deg(v)} J - I$$

to vertex v and the transition matrix of the walk is

$$U = R \bigoplus_{v \in V(G)} \left(\frac{2}{\deg(v)} J - I \right).$$

Below we give a more detailed explanation about how we define U, which helps us to build a connection between Grover's walk and bipartite walks.

Given a graph G, we can give directions to the edges of G such that the arc set of G is

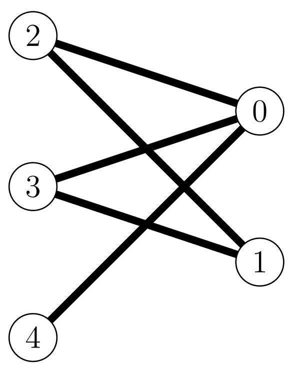
$$\mathcal{A} = \big\{(a,b),(b,a) \mid \{a,b\} \in E(G)\big\}.$$

If $\alpha = (x,y)$, we define $\alpha^{-1} = (y,x)$. Define a matrix $D \in \mathbb{C}^{V \times \mathcal{A}}$ such that

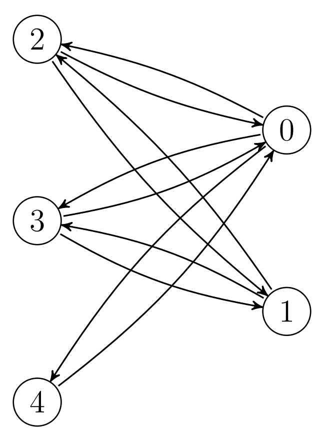
$$D_{x,\alpha} = \frac{1}{\sqrt{\deg(x)}} \delta_{x,t(\alpha)}.$$

Then $D^*D \in \mathbb{C}^{\mathcal{A}\times\mathcal{A}}$ is given by

$$(D^*D)_{\alpha,\beta} = \begin{cases} \frac{1}{\deg(t(\alpha))}, & \text{if } t(\alpha) = t(\beta); \\ 0, & \text{otherwise.} \end{cases}$$



(a) Graph G



(b) Directed Graph $\overrightarrow{G}$

Let $R \in \mathbb{C}^{\mathcal{A}\times\mathcal{A}}$ denote the arc-reversal matrix, i.e.,

$$R_{\alpha,\beta} = \delta_{\alpha,\beta^{-1}}.$$

The transition matrix of the *Grover's walk* defined on G is

$$U_{\mathrm{GW}} = R(2D^*D - I).$$

4.4 Grover's walk is a special case of bipartite walk

Given a graph G, we define a new graph by subdividing every edge of G exactly once and we call the resulting graph *the subdivision graph* of G, denoted by $S(G)$. For example, the graph in Figure 4.2 is the subdivision graph of the graph in Figure 4.1a.

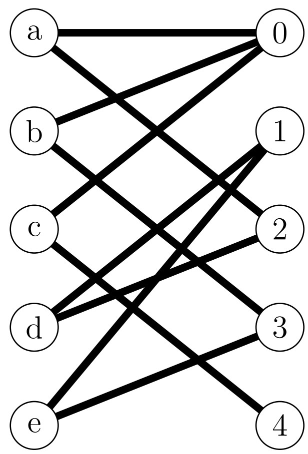


Figure 4.2: The subdivision graph of G

Now we are going to show the transition matrix of the Grover's walk defined on G is exactly the same as the transition matrix of the bipartite walk defined on the subdivision graph of G.

Given a graph G, its subdivision graph $S(G)$ is a bipartite graph with parts

$$\begin{aligned} C_0 &= V(S(G)) \backslash V(G) = \{a_0, a_1, \cdots, a_m\}, \\ C_1 &= V(G) = \{v_1, v_2, \cdots, v_n\}. \end{aligned}$$

For the subdivision graph shown in Figure 4.2, its parts are

$$C_0 = \{a, b, c, d, e, \}, \quad C_1 = \{1, 2, 3, 4\}.$$

Following the notation and the construction described in Section 2.1, the transition matrix of the bipartite walk on $S(G)$ is

$$U_{S(G)} = (2P_{S(G)} - I)(2Q_{S(G)} - I).$$

Note that the rows and columns of U_{BW} are indexed by the edges of $S(G)$ and rows and columns of U_{GW} are indexed by arcs of $\overrightarrow{G}$.

Also, note that every edge $(v_i, v_j) \in E(G)$ is subdivided into two edges $(v_i, a_s), (v_j, a_s)$ in $S(G)$ for some $a_s \in C_0$. We also have that for every edge $(v_i, v_j) \in E(G)$, it contributes two arcs $(v_i, v_j), (v_j, v_i)$ in $\mathcal{A}$ of $\overrightarrow{G}$. This shows there is a bijection between $E\left(S(G)\right)$ and $\mathcal{A}$

For each vertex $i \in C_1\left(S(G)\right)$, we have $\deg_{S(G)}(i) = \deg_G(i)$ and $C_1\left(S(G)\right) = V(G)$. Using the bijection between $E\left(S(G)\right)$ and $\mathcal{A}$, we can index edges of $S(G)$ and arcs of $\overrightarrow{G}$ such that

$$Q_{S(G)} = D^* D.$$

For each vertex $a' \in C_0\left(S(G)\right)$, we have $\deg_{S(G)}(a') = 2$. Two edges $(v_i, a'), (a', v_j)$ of $S(G)$ share a vertex in $C_0\left(S(G)\right)$ if and only if $(v_i, v_j) \in E(G)$. We index rows and columns of P using the same indexing as we do for Q and we also index rows and columns of R use the same indexing as we do for $D^* D$. Consequently, we get

$$2P_{S(G)} - I = R.$$

Thus, we have proved the following theorem.

4.4.1 Theorem. *Given a graph G, let $U_{BW}\left(S(G)\right)$ be the transition matrix of the bipartite walk defined on $S(G)$ and let $U_{GW}\left(G\right)$ be the transition matrix of Grover's walk defined on G. Then*

$$U_{BW}\left(S(G)\right) = U_{GW}\left(G\right). \qquad \square$$

4.5 One step of the bipartite walk on G is two steps of Grover's walk on G

Given a bipartite graph G, bipartite walks and Grover's walk are two models that one can apply to G to define a discrete quantum walk over G. In previous section, we have shown that Grover's walk on a graph and the bipartite walk on its subdivision graph are equivalent. In this section, we are going to show that actually bipartite walk model actually has an advantage over Grover's walk, i.e., every $2k$-th power of the transition matrix of Grover's walk on G is a direct sum of k-th power of the transition matrix of the bipartite walk defined on the same graph.

Note that every edge of $S(G)$ has one of its ends in $V(G)$. We index rows and columns of $U_{BW}(S(G))$ such that the first half of the the rows and columns are indexed by the edges with one end in the color class C_1 of G and the others are indexed by edges with one end in the color class C_0 of G. For example, consider the bipartite walk defined on the subdivision graph $S(G)$ shown in Figure 4.2. We can index the rows and columns of $Q_{S(G)}$ such that $Q_{S(G)}$ has the form as below.

$$
\begin{array}{c}
\\
(a,0)\\ (b,0)\\ (c,0)\\ (d,1)\\ (e,1)\\ (a,2)\\ (b,3)\\ (c,4)\\ (d,2)\\ (e,3)
\end{array}
\begin{array}{c}
\begin{array}{cccccccccc}
(a,0) & (b,0) & (c,0) & (d,1) & (e,1) & (a,2) & (b,3) & (c,4) & (d,2) & (e,3)
\end{array}\\
\left(\begin{array}{ccccc|ccccc}
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
\frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0\\
0 & 0 & 0 & \frac{1}{2} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0\\
\hline
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2}\\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0\\
0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2} & 0\\
0 & 0 & 0 & 0 & 0 & 0 & \frac{1}{2} & 0 & 0 & \frac{1}{2}
\end{array}\right)
\end{array}
$$

Let P_G and Q_G denote the projections on two color classes of G as we defined in Section 2.1. Then we can have that

$$Q_{S(G)} = \begin{pmatrix} Q_G & 0 \\ 0 & P_G \end{pmatrix}.$$

It follows that

$$U_{BW}(S(G)) = U_{GW}(G) = R\begin{pmatrix} 2Q_G - I & 0 \\ 0 & 2P_G - I \end{pmatrix} = \begin{pmatrix} 0 & 2P_G - I \\ 2Q_G - I & 0 \end{pmatrix}.$$

Following directly from the equation above, we have the following theorem.

4.5.1 Theorem. *Let G be a bipartite graph. Let U_{BW} and U_{GW} be the transition matrices of the bipartite walk and Grover's walk defined on G*

respectively. Then for any non-negative integer k, we have that

$$U_{GW}{}^{2k} = \begin{pmatrix} U_{BW}^k & 0 \\ 0 & U_{BW}^T{}^k \end{pmatrix}. \qquad \square$$

The following corollary shows that the period of a periodic Grover's walk has to be even and the period of a periodic bipartite walk on G is half of the period of the periodic Grover's walk defined on the same graph.

4.5.2 Corollary. *Let G be a bipartite graph. The bipartite walk defined on G is periodic with τ if and only if Grover's walk defined on G is periodic with period 2τ for some integer τ.*

Proof. Let U_{BW} and U_{GW} be the transition matrices of the bipartite walk and Grover's walk defined on G respectively. By Theorem 4.5.1, we can see that for any non-negative integer m,

$$U_{GW}^{2m} = \begin{pmatrix} U_{BW}^m & 0 \\ 0 & \left(U_{BW}^T\right)^m \end{pmatrix}$$

and for odd positive integer i, we have

$$U_{GW}^{i} = \begin{pmatrix} 0 & (2P-I)U_{BW}^{i-1} \\ (2Q-I)\left(U_{BW}^T\right)^{i-1} & 0 \end{pmatrix}.$$

It follows immediately that Grover's walk on G cannot have odd period.

If the bipartite walk defined on G is periodic with period τ, then it is easy to see that Grover's walk is periodic. Assume Grover's walk on G has period $2k$ for some integer k. If $2k < 2\tau$, then

$$U_{BW}^k = I,$$

which contradicts that U_{BW} has period τ. Thus, Grover's walk on G is periodic with period 2τ.

Now assume that the Grover's walk is periodic with period $2k$. By Theorem 4.5.1, the bipartite walk is periodic with period k. $\square$

Chapter 5

Periodicity of Bipartite Walks

In this chapter, we study periodicity of bipartite walks. Periodicity is one of the interesting phenomena in quantum walks. Periodic quantum walks aid in the design of new quantum algorithms in quantum cryptography. In [30], Panda and Benjamin use two chaotic quantum walks to get a periodic quantum walk with transition matrix U. Using the fact the walk is periodic, i.e., there exists an integer k such that $U^k = I$, they show that the message can be decrypted with a given public key. Periodic quantum walks are also of interest in development of quantum chaos control theory [36]. Periodicity of discrete quantum walks is studied using many different discrete quantum walk models [5,23]. In [29], Kubota studies the periodicity of Grover's walks on regular bipartite graphs with at most five distinct eigenvalues. In that paper, Kubota proves the following theorem:

5.0.1 Theorem (Theorem 3.3, Theorem 4.1 in [29])**.** *Let Γ be a bipartite d-regular graph with the A-spectrum $\{[\pm d]^1, [\pm\theta]^a, [0]^b\}$, where $a \geq 0$ and $b \geq 0$. Then Γ is periodic with respect to Grover's walk if and only if one of the following holds:*

(a) if $a = 0, b = 0$, then G is a complete bipartite graph $K_{d,d}$,

(b) if $a \geq 1, b = 0$, then G is C_6,

(c) if $a \geq 1, b \geq 1$, then $\theta \in \left\{\frac{\sqrt{2}}{2}d, \frac{\sqrt{3}}{2}d, \frac{1}{2}d\right\}$ and d must be even. □

In this chapter, we give a necessary and sufficient condition for a state of a bipartite walk to be periodic. A periodic walk is a quantum walk all of whose states are periodic. Results from algebraic number theory are the main tools we use. We derive a characterization of periodic bipartite walks on biregular graph squares of whose eigenvalues are algebraic integers with degree at most two. We have shown in Section 4.4 that Grover's walk on a graph is the same as the bipartite walk on its subdivision graph. In the last section, we use the characterization of periodic bipartite walks to extend Theorem 5.0.1.

The results in this chapter can be found in my paper [8].

5.1 Periodic states

Given a graph G, let U denote the transition matrix of the bipartite walk defined over G. Note that the rows and columns of U are indexed by the edges of G.

A *density* matrix is a positive semidefinite matrix ρ with $\operatorname{tr}(\rho) = 1$. We can use a density matrix to represent a state of a discrete walk. Let e_a denote the standard basis vector in $\mathbb{C}^{E(G)}$ indexed by the edge a in graph G. The matrix

$$D_a = e_a e_a^T$$

is a *state* associated with edge a of G. If a walker starts at state D_a, after k steps, the walker is at the state

$$D_a(k) = U^k D_a U^{-k}.$$

We say a state a is *periodic* if and only if there exist a positive integer τ such that

$$D_a(\tau) = U(\tau) D_a U(-\tau) = D_a.$$

Now, given a bipartite walk governed by transition matrix U, we are going to derive necessary and sufficient conditions for a state to be periodic in terms of the eigenvalues of U.

If the spectral decomposition of U is $\sum_r e^{i\theta_r} E_r$, then the *eigenvalue support* of a state D is the set

$$\left\{ \left(e^{i\theta_r}, e^{i\theta_s}\right) : E_r D E_s \neq 0 \right\}.$$

Equivalently, if a state is represented by a unit vector e_a, then the eigenvalue support of the state e_a is the set

$$\left\{ e^{i\theta_r} : E_r e_a \neq \mathbf{0} \right\}.$$

5.1.1 Theorem. *Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix of a bipartite walk. State D_a is periodic if and only if $\theta_r, \theta_s \in \mathbb{Q}\pi$ for all $(e^{i\theta_r}, e^{i\theta_s})$ in the eigenvalue support of D_a.*

Proof. Since D_a is periodic, there is a positive integer τ such that

$$D_a(\tau) = \sum_{r,s} e^{i\tau(\theta_r - \theta_s)} E_r D_a E_s = D_a.$$

Since

$$D_a = \sum_{r,s} E_r D_a E_s,$$

we must have

$$e^{i\tau(\theta_r - \theta_s)} E_r D_a E_s = E_r D_a E_s$$

for every $e^{i\theta_r}, e^{i\theta_s}$. In particular, the pair $(e^{i\theta_r}, e^{-i\theta_r})$, is in the eigenvalue support of D_a. Then by taking $\theta_s = -\theta_r$, we have that

$$E_r D_a \overline{E_r} = e^{2\tau\theta_r i} E_r D_a \overline{E_r}.$$

Since entries of $E_r D_a \overline{E_r} = (E_r e_a)\overline{(E_r e_a)}$ are the norm squares of entries of $E_r e_a$, they are real and non-negative. We must have that

$$e^{2\tau\theta_r i} = 1,$$

which implies that

$$2\tau\theta_r = 2m_r\pi,$$

for some integer m_r. Therefore,

$$\theta_r = \frac{m_r}{\tau}\pi \in \mathbb{Q}\pi.$$

□

5.2 Periodic walks

Let U denote the transition matrix of the bipartite walk defined on graph G. We say U is a *periodic walk* if every edge state of U is periodic, i.e., there exists a positive integer k such that

$$U^k = I.$$

In this case, sometimes we also say the graph is periodic when the context is clear.

The following theorem is essentially the same as Lemma 3.2 in [29].

5.2.1 Theorem. *Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix of the bipartite walk defined over graph G. If the bipartite walk is periodic, then $2\cos k\theta_r$ is an algebraic integer for any non-negative integer k.*

Proof. If G is periodic with period t, i.e.,

$$U^t = I,$$

eigenvalue $e^{i\theta_r}$ of U is a root of $x^t - 1$ and this implies that $e^{i\theta_r}$ is an algebraic integer. Then for any non-negative integer k, we have that

$$\left(e^{i\theta_r}\right)^k + \left(e^{-i\theta_r}\right)^k = 2\cos k\theta_r$$

is an algebraic integer. □

Using the theorem above, we can derive a necessary condition for a graph being periodic. Computationally this provides an easy way for us to determine when a graph is not periodic.

5.2.2 Theorem. *Let G be a periodic bipartite graph. Then* $\operatorname{tr}(U^k) \in \mathbb{Z}$ *for any integer k.*

Proof. Since U is a rational matrix, we know $\operatorname{tr}(U) \in \mathbb{Q}$. On the other hand,

$$\operatorname{tr}(U^k) = \sum_r e^{ik\theta_r} = \sum_r 2\cos k\theta_r.$$

By Theorem 5.2.1, we know $2\cos k\theta_r$ is an algebraic integer for any integer k. So $\operatorname{tr}(U^k)$ is an algebraic integer. Hence, when G is periodic, we must have that

$$\operatorname{tr}(U^k) \in \mathbb{Z}$$

for any integer k. □

Using the necessary condition for periodicity stated above, we can easily see that the graph shown in Figure 2.1 is not periodic, since the transition matrix has trace $-\frac{1}{3}$.

5.3 Periodic walks on biregular graphs

In this section, we study periodic bipartite walks defined on biregular graphs. We show that if a biregular graph G has eigenvalues whose squares are algebraic integers with degree at most two, there is a characterization of periodicity of bipartite walks in terms of spectrum of G.

The reason why we choose to look at bipartite walks on biregular graphs is that if the underlying bipartite graph G of a bipartite walk is biregular, we can show that the spectrum of $A(G)$ determines the spectrum of U.

In Section 2.2, we have shown that the spectrum of $\widehat{C}\widehat{C}^T$ determines the spectrum of U. Now we are going to show that the spectrum of $A(G)$ determines the spectrum of $\widehat{C}\widehat{C}^T$ when G is a biregular graph.

5.3.1 Theorem. *Let G be a biregular graph with degree (d_0, d_1) and U is the transition matrix of the bipartite walk defined over G. Then for every complex eigenvalue $e^{i\theta_r}$ of U, we have that*

$$\cos\theta_r = 2\frac{\lambda_r^2}{d_0 d_1} - 1,$$

where λ_r is an eigenvalue of $A(G)$.

Proof. Recall that in Section 2.1, we define

$$C = P_1^T P_0.$$

Using the definitions of P, Q, it is not hard to see that

$$A(G) = \begin{pmatrix} \mathbf{0} & C \\ C^T & \mathbf{0} \end{pmatrix}.$$

Again in Section 2.1 we define that $\widehat{C} = \widehat{P}_1^T \widehat{P}_0$. If G is biregular with degree (d_0, d_1), we have that

$$\widehat{C} = \frac{1}{\sqrt{d_0 d_1}} C.$$

It follows that

$$A^2 = \begin{pmatrix} \mathbf{0} & C \\ C^T & \mathbf{0} \end{pmatrix} \begin{pmatrix} \mathbf{0} & C \\ C^T & \mathbf{0} \end{pmatrix} = \begin{pmatrix} CC^T & \mathbf{0} \\ \mathbf{0} & C^T C \end{pmatrix},$$

which implies that

$$\operatorname{Spec}(A^2) = \operatorname{Spec}(CC^T) \cup \operatorname{Spec}(C^T C). \tag{5.3.1}$$

Theorem 2.2.6 states that for every eigenvalue μ_r of $\widehat{C}\widehat{C}^T$ with $\mu_r \in (0, 1)$, we have that

$$\cos\theta_r = 2\mu_r - 1$$

for every complex eigenvalue $e^{i\theta_r}$ of U. Since G is biregular with degree (d_0, d_1), we have that

$$\frac{1}{d_0 d_1} C C^T = \widehat{C}\widehat{C}^T.$$

For every complex eigenvalue $e^{i\theta_r}$ of U, by Equation 5.3.1, we have that

$$\cos\theta_r = 2\frac{\lambda_r^2}{d_0 d_1} - 1,$$

where λ_r is an eigenvalue of $A(G)$. □

The following two results from algebraic number theory are important tools for us. We use them to derive a characterization of periodicity of bipartite walks on biregular graphs squares of whose eigenvalues are algebraic integer with degree at most two.

5.3.2 Lemma (Theorem 3.3 in [35])**.** *Let $\alpha \in [0,1]$. Assume that $\frac{1}{\pi}\arccos\alpha = \frac{2k}{n}, k \in \mathbb{Z}, n \in \mathbb{N}, \gcd(k,n) = 1$. Then*

(i) the number $2\alpha = 2\cos\frac{2k\pi}{n}$ is an algebraic integer of degree one if and only if $n = 1, 2, 3, 4, 6$; in such cases, all the values taken by α are

$$1 = \cos 0 = -\cos\pi, \quad 0 = \cos\frac{2\pi}{4} = \cos\frac{6\pi}{4},$$
$$\frac{1}{2} = \cos\frac{2\pi}{6} = \cos\frac{10\pi}{6} = -\cos\frac{2\pi}{3} = -\cos\frac{4\pi}{3};$$

(ii) the number $2\alpha = 2\cos\frac{2k\pi}{n}$ is an algebraic integer of degree two if and only if $n = 5, 8, 10, 12$; in such cases, all the values taken by α are

$$\frac{\sqrt{5}-1}{4} = \cos\frac{2\pi}{5} = \cos\frac{8\pi}{5} = -\cos\frac{6\pi}{10} = -\cos\frac{14\pi}{10},$$
$$\frac{\sqrt{5}+1}{4} = -\cos\frac{4\pi}{5} = -\cos\frac{6\pi}{5} = \cos\frac{2\pi}{10} = \cos\frac{18\pi}{10},$$
$$\frac{\sqrt{2}}{2} = \cos\frac{2\pi}{8} = \cos\frac{14\pi}{8} = -\cos\frac{6\pi}{8} = -\cos\frac{10\pi}{8},$$
$$\frac{\sqrt{3}}{2} = \cos\frac{2\pi}{12} = \cos\frac{22\pi}{12} = -\cos\frac{10\pi}{12} = -\cos\frac{14\pi}{12}.$$

□

5.3.3 Lemma (Proposition 2.34 in [25]). *Suppose that m is a square-free integer (i.e., not divisible by the square of any prime). Let Ω denote the set of algebraic integer. Then*

$$\Omega \cap \mathbb{Q}(\sqrt{m}) = \begin{cases} \{p + q\sqrt{m} : p, q \in \mathbb{Z}\} & \text{if } m \equiv 2, 3 \pmod 4, \\ \{p + \frac{1+\sqrt{m}}{2} q : p, q \in \mathbb{Z}\} & \text{if } m \equiv 1 \pmod 4. \end{cases} \qquad \square$$

The definition of a periodic walk says that if the graph is periodic, every state of G is periodic, which implies that Theorem 5.1.1 applies to all the eigenvalues of G.

5.3.4 Theorem. *Let G be a biregular graph with degree (d_0, d_1). Assume that squares of eigenvalues λ_r of $A(G)$ are algebraic integers with degree at most two. The bipartite walk defined over G is periodic if and only if every eigenvalue λ_r of $A(G)$ satisfies that*

(a) if λ_r^2 is an algebraic integer of degree one, then $d_0 d_1 \equiv 0 \pmod 4$ and

$$\lambda_r^2 \in \left\{ \frac{1}{2} d_0 d_1,\ \frac{3}{4} d_0 d_1,\ \frac{1}{4} d_0 d_1,\ 0,\ d_0 d_1 \right\};$$

(b) if λ_r^2 is an algebraic integer of degree two, then

$$\lambda_r^2 \in \left\{ \left(\frac{1}{2} \pm \frac{\sqrt{2}}{4}\right) d_0 d_1,\ \left(\frac{1}{2} \pm \frac{\sqrt{3}}{4}\right) d_0 d_1,\ \frac{5 \pm \sqrt{5}}{8} d_0 d_1,\ \frac{3 \pm \sqrt{5}}{8} d_0 d_1 \right\}.$$

Moreover, λ_r^2 comes in algebraic conjugate pairs.

Proof. By Theorem 5.1.1, the bipartite walk defined on G is periodic if and only if $\frac{\theta_r}{\pi} \in \mathbb{Q}$ for all eigenvalues $e^{i\theta_r}$ of U. It is easy to check that the condition stated in the theorem is sufficient. Now we are going to prove it is also necessary.

By Theorem 5.2.1, if G is periodic, then $2\cos\theta_r$ is an algebraic integer. As shown in Theorem 5.3.1, for every eigenvalue λ_r of $A(G)$,

$$\cos\theta_r = 2\frac{\lambda_r^2}{d_0 d_1} - 1.$$

By assumption, the number λ_r^2 is an algebraic integer of degree at most two, which is the same as

$$\lambda_r^2 = a + b\sqrt{m_r}$$

for some square-free integer m_r and $a, b \in \mathbb{Q}$. By Lemma 5.3.2, we know that G is periodic if and only if

(a) when $b = 0$, i.e., $\lambda_r^2 \in \mathbb{Q}$,

$$\cos\theta_r \in \left\{0, \pm 1, \pm\frac{1}{2}\right\};$$

(b) when $\lambda_r^2 = a + b\sqrt{m_r}$ for some square-free integer m_r and non-zero $a, b \in \mathbb{Q}$,

$$\cos\theta_r \in \left\{ \pm\frac{\sqrt{2}}{2}, \pm\frac{\sqrt{3}}{2}, \pm\frac{\sqrt{5}+1}{4}, \pm\frac{\sqrt{5}-1}{4}\right\}.$$

First consider the case when $\lambda_r^2 \in \mathbb{Q}$. If

$$\cos\theta = 2\frac{\lambda^2}{d_0 d_1} - 1 = 0,$$

we have that

$$\lambda^2 = \frac{1}{2} d_0 d_1.$$

If

$$\cos\theta = 2\frac{\lambda^2}{d_0 d_1} - 1 = 1,$$

we have that

$$\lambda^2 = d_0 d_1,$$

which is guaranteed since the largest eigenvalue of $A(G)$ is $\sqrt{d_0 d_1}$. Similarly, when $\cos\theta = 2\frac{\lambda^2}{d_0 d_1} - 1 = -1$, we have that $\lambda_r = 0$.

Consider the case when

$$\cos\theta = 2\frac{\lambda_r^2}{d_0 d_1} - 1 = \frac{1}{2},$$

we have that

$$\frac{\lambda_r^2}{d_0 d_1} = \frac{3}{4}.$$

Similarly, when $\cos\theta = -\frac{1}{2}$, we have that $\lambda_r^2 = \frac{1}{4}d_0d_1$. Note that if an algebraic integer is rational, then it is integer. Thus, if $b = 0$, we require $d_0d_1 \equiv 0 \pmod 4$.

Now consider the case when $\lambda_r^2 = a + b\sqrt{m_r}$ for some square-free integer m_r and non-zero $a, b \in \mathbb{Q}$. Assume

$$\cos\theta = 2\left(\frac{\lambda_r^2}{d_0d_1} - 1\right) = \pm\frac{\sqrt{2}}{2}.$$

Using Lemma 5.3.3, we assume that

$$\lambda_r^2 = p + q\sqrt{2},$$

where p, q are both non-zero integers and

$$\cos\theta = 2\frac{(p + q\sqrt{2})}{d_0d_1} - 1 = \pm\frac{\sqrt{2}}{2}.$$

Then we have that

$$\frac{2p}{d_0d_1} - 1 = 0, \quad \frac{2q}{d_0d_1} = \pm\frac{1}{2}.$$

Combining both equations above, we have that

$$p = \pm 2q = d_0d_1$$

and

$$\lambda^2 = \left(1 \pm \frac{\sqrt{2}}{2}\right)p = \left(\frac{1}{2} \pm \frac{\sqrt{2}}{4}\right)d_0d_1.$$

When

$$2\frac{\lambda_r^2}{d_0d_1} - 1 = \pm\frac{\sqrt{3}}{2},$$

by Lemma 5.3.3, we assume that

$$\lambda_r^2 = p + q\sqrt{3}.$$

Then using the similar argument as previous case, we have that

$$\lambda^2 = (1 \pm \frac{\sqrt{3}}{2})p = \left(\frac{1}{2} \pm \frac{\sqrt{3}}{4}\right)d_0d_1.$$

Now, consider the case when

$$\cos\theta_r = 2\frac{\lambda_r^2}{d_0d_1} - 1 = \pm\frac{\sqrt{5}+1}{4}.$$

This implies that

$$\lambda_r^2 = p + \frac{1+\sqrt{5}}{2}q,$$

where p, q are both non-zero integers. So

$$\frac{2}{d_0d_1}\left(p + \frac{1+\sqrt{5}}{2}q\right) - 1 = \pm\frac{1+\sqrt{5}}{4}.$$

This implies that

$$\frac{2}{d_0d_1}(p+\frac{q}{2}) - 1 = \frac{1}{4}, \quad \frac{q}{d_0d_1} = \frac{1}{4}$$

or

$$\frac{2}{d_0d_1}(p+\frac{q}{2}) - 1 = -\frac{1}{4}, \quad \frac{q}{d_0d_1} = -\frac{1}{4}.$$

Combining two equations of either case above, we have

$$p = \pm 2q = \frac{1}{2}d_0d_1,$$

and consequently,

$$\lambda_r^2 = \frac{5+\sqrt{5}}{8}d_0d_1 \text{ or } \frac{3-\sqrt{5}}{8}d_0d_1$$

when $p = 2q$ and $p = -2q$ respectively. Similarly, when $\cos\theta_r = \pm\frac{\sqrt{5}-1}{4}$, we have

$$p = -3q = \frac{3}{4}d_0d_1, \text{ or } p = q = \frac{1}{4}d_0d_1,$$

and consequently,

$$\lambda_r^2 = \frac{5-\sqrt{5}}{8}d_0d_1, \text{ or } \lambda_r^2 = \frac{3+\sqrt{5}}{8}d_0d_1.$$

We can view λ_r^2 as eigenvalues of $A(G)^2$. So λ_r^2 comes in algebraic conjugate pairs. □

The characterization we derived above only depends on the spectrum of the underlying graph. The possible spectrum for a periodic bipartite walk shown in the theorem above is determined by the degrees of the underlying biregular graph.

5.4 Spectrum of G determines the spectrum of $S(G)$

We have shown in Section 4.4 that given a graph G, the transition matrix of Grover's walk on G is the same as the transition matrix of the bipartite walk on the subdivision graph of G. In the next section, we will use the characterization of periodic biparite walks (Theorem 5.3.4) to study the periodicity of Grover's walks. But before that, we need to understand the relation between the spectrum of a graph and the spectrum of its subdivision graph, which is what this section about.

Let G be a regular graph. In this section, we are going to give an explicit formula for the eigenvalues of $A(S(G))$ in terms of eigenvalues of $A(G)$. To do this, first we show that eigenvalues of the line graph $L(G)$ of G determine eigenvalues of $S(G)$. Then since G is regular, eigenvalues of $L(G)$ are determined by eigenvalues of G, which helps us build a connection between eigenvalues of G and eigenvalues of $S(G)$.

5.4.1 Lemma. *Given a graph G, the value $\lambda - 2$ is an eigenvalue of $L(G)$ if and only if $\pm\sqrt{\lambda}$ are eigenvalues of $S(G)$.*

Proof. Let B be the vertex-edge incidence matrix of G and Δ be the degree matrix of G . We have that

$$BB^T = \Delta(G) + A(G), \quad B^T B = A(L(G)) + 2I.$$

The adjacency matrix of the subdivision graph $S(G)$ of G is

$$A(S(G)) = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}.$$

Let x be an eigenvector of $B^T B$ such that $B^T Bx = \lambda x$, then

$$\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} Bx \\ \sqrt{\lambda}x \end{pmatrix} = \begin{pmatrix} \sqrt{\lambda}Bx \\ \lambda x \end{pmatrix} = \sqrt{\lambda} \begin{pmatrix} Bx \\ \sqrt{\lambda}x \end{pmatrix},$$

which implies that $\begin{pmatrix} Bx \\ \sqrt{\lambda}x \end{pmatrix}$ is an eigenvector of $\begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix}$.

On the other hand, we also have that $\begin{pmatrix} x & y \end{pmatrix}^T$ is an eigenvector of $A(S(G))$ with eigenvalue μ, which implies that

$$A\left(S(G)\right)^2 \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} 0 & B \\ B^T & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} BB^T & 0 \\ 0 & B^T B \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \lambda^2 \begin{pmatrix} x \\ y \end{pmatrix}$$

if and only if

$$BB^T x = \mu^2 x, \quad B^T By = \mu^2 y,$$

for some λ. □

The following lemma is a standard result from algebraic graph theory and this helps us to derive the relation between eigenvalues of $A(G)$ and $A(S(G))$ when G is a regular graph.

Let G be a graph and we let $\Phi(G, x)$ denote the characteristic polynomial of $A(G)$.

5.4.2 Lemma (Lemma 8.2.5 in [18])**.** *Let G be a regular graph of valency d with n vertices and e edges and let LG be the line graph of G. Then*

$$\phi(LG, x) = (x+2)^{e-n}\phi(G, x-d+2).$$ □

Since -2 is always an eigenvalue of $L(G)$, zero is always an eigenvalue of $S(G)$.

5.4.3 Corollary. *Let G be a d-regular graph. Then λ is an eigenvalue of G with $\lambda \neq -d$ if and only if $\pm\sqrt{\lambda + d}$ is a non-zero eigenvalue of $S(G)$.*

Proof. Lemma 5.4.2 states that if λ is an eigenvalue of $A(G)$, then $\lambda+d-2$ is an eigenvalue of $L(G)$. It follows from Lemma 5.4.1 that for every eigenvalue λ of G, we have that $\pm\sqrt{\lambda + d}$ are eigenvalues of $S(G)$. □

5.5 Periodic Grover's walks on regular graphs

We have shown in Section 4.4 that given a graph G, the transition matrix of Grover's walk on G is the same as the transition matrix of the bipartite walk on the subdivision graph of G. If G is a k-regular graph, then the subdivision graph $S(G)$ of G is a $(2, k)$-biregular graph. Using Theorem 5.3.4, we can give a characterization of periodic Grover's walks on regular graphs whose eigenvalues are algebraic integers with degree at most two.

In this section, given a regular bipartite graph G, we consider the bipartite walk on its subdivision graph $S(G)$, i.e., the Grover's walk on G as shown in Section 4.4. We give a characterization of periodic bipartite walk on $S(G)$ when all the eigenvalues of G satisfy that their squares are algebraic integers of degree at most two. We give a simpler proof of the main results in [29]. We also show that given a regular bipartite graph G, the bipartite walk on G is periodic if and only if Grover's walk on G is periodic.

5.5.1 Corollary. *Let G be a d-regular graph, all of whose eigenvalues are algebraic integers of degree at most two in the form of*

$$\lambda_r = a + b\sqrt{m_r}$$

for some $a, b \in \mathbb{Q}$ and square-free integer m_r. Let $S(G)$ denote the subdivision graph of G. The bipartite walk defined over $S(G)$ is periodic if and only if for every eigenvalue λ_r of G,

(a) if $b = 0$, $\lambda_r \in \left\{0, \pm d, \pm\frac{1}{2}d\right\}$;

(b) if $b \neq 0$, $\lambda_r \in \left\{\pm\frac{\sqrt{2}}{2}d, \pm\frac{\sqrt{3}}{2}d, \frac{1\pm\sqrt{5}}{4}d, \frac{-1\pm\sqrt{5}}{4}d\right\}$.

Note that eigenvalues of G come in algebraic conjugate pairs.

Proof. By assumption, λ_G, an eigenvalue of G, is an algebraic integer of degree at most two, so by Corollary 5.4.3, the eigenvalue $\lambda_{S(G)}$ of $S(G)$ satisfies that

$$\lambda_{S(G)}^2 = \lambda_G + d.$$

Thus, we know that $\lambda_{S(G)}^2$ is an algebraic integer with degree at most two. We can write

$$\lambda_{S(G)}^2 = a + b\sqrt{m_r}$$

for some square-free integer m_r and $a, b \in \mathbb{Q}$.

Graph $S(G)$ is biregular with degree $(2, d)$. By Theorem 5.1.1, the bipartite walk defined over $S(G)$ is periodic if and only if for every eigenvalue $\lambda_{S(G)}$ of $S(G)$, it satisfies that

(a) when $b = 0$, $\lambda_{S(G)}^2 \in \left\{d, \frac{3}{2}d, \frac{1}{2}d, 0, 2d\right\}$ and $d \equiv 0 \pmod 2$;

(b) when $b \neq 0$, $\lambda_{S(G)}^2 \in \left\{\left(1 \pm \frac{\sqrt{2}}{2}\right)d, \left(1 \pm \frac{\sqrt{3}}{2}\right)d, \frac{\sqrt{5}\pm 5}{4}d, \frac{3\pm\sqrt{5}}{4}d\right\}$.

Using Corollary 5.4.3, we see that when

$$\lambda_{S(G)}^2 = \frac{\sqrt{5}+5}{4}d \text{ or } \frac{3-\sqrt{5}}{4}d,$$

we get that

$$\lambda_G = \frac{1+\sqrt{5}}{4}d \text{ or } -\frac{1+\sqrt{5}}{4}d$$

respectively. Similarly, when

$$\lambda^2_{S(G)} = \frac{5-\sqrt{5}}{4}d \text{ or } \frac{3+\sqrt{5}}{4}d,$$

we get

$$\lambda_G = -\frac{\sqrt{5}-1}{4}d \text{ or } \frac{\sqrt{5}-1}{4}d$$

respectively. The rest of the statement of this corollary also follows directly from Corollary 5.4.3. □

If a graph has at most five distinct eigenvalues, then every eigenvalue is an algebraic integer of degree at most two. So we can see that Corollary 5.5.1 extends Theorem 5.0.1 by Kubota. In particular, we get rid of the constrain that the graph has to be bipartite in Theorem 5.0.1.

Now we restrict Corollary 5.5.1 to the case when G is a regular bipartite graph with at most five distinct eigenvalues to give a simpler proof of Theorem 5.0.1 by Kubota. The proof we provide here is using results on periodic bipartite walks.

5.5.2 Corollary (Theorem 3.3, Theorem 4.1 in [29])**.** *Let G be a regular bipartite graph G with at most five distinct eigenvalues. The bipartite walk defined on $S(G)$ is periodic if and only if one of the following holds:*

(a) G is a complete bipartite graph $K_{d,d}$,

(b) G is C_6,

(c) G has exactly five eigenvalues $\left\{0, \pm\theta, \pm d\right\}$ with $\theta \in \left\{\frac{\sqrt{2}}{2}d, \frac{\sqrt{3}}{2}d, \frac{1}{2}d\right\}$ and d must be even.

Proof. A regular bipartite graph that has two or three distinct eigenvalues is a complete bipartite graph. Now consider the case when G has exactly four distinct eigenvalues. Cvetković et al. in [14, Page 116] prove that a connected bipartite regular graph with four distinct eigenvalues must be the incidence graph of a symmetric 2-(v, d, λ) design and its spectrum is

$$[d]^1, \quad [\sqrt{d-\lambda}]^{v-1}, \quad [-\sqrt{d-\lambda}]^{v-1}, [-d]^1.$$

Since $d-\lambda$ must be an integer, by Corollary 5.5.1, the possible values of the second largest eigenvalue of $A(G)$ are $\left\{\frac{\sqrt{2}}{2}d, \frac{\sqrt{3}}{2}d, \frac{1}{2}d\right\}$. Thus, one of the following three holds:

$$\lambda = d - \frac{1}{4}d^2, \quad \lambda = d - \frac{3}{2}d^2, \quad \lambda = d - \frac{1}{2}d^2.$$

For a positive integer λ, the only equation that has an integer solution is $\lambda = d - \frac{1}{4}d^2$ and the solution is $d = 2$. The incidence graph of a symmetric design has diameter three. Since $d = 2$ here, the only feasible graph is C_6.

If G has five eigenvalues, then d must be even and the eigenvalues must be $\{\pm d, \pm\theta, 0\}$. By Corollory 5.5.1, we know the eigenvalues of G comes in algebraic conjugate pairs. Since G has only five eigenvalues, we must have $\theta \in \left\{\frac{\sqrt{2}}{2}d, \frac{\sqrt{3}}{2}d, \frac{1}{2}d\right\}$. A rational algebraic integer is an integer, so, if $\theta = \frac{1}{2}d$, then d must be even. If $\theta \in \{\frac{\sqrt{3}}{2}d, \frac{\sqrt{2}}{2}d\}$, by Lemma 5.3.3, then d must be even. □

One can refer to the tables at the end of [29] for examples of d-regular bipartite graphs with exactly five eigenvalues $\left\{0, \pm\theta, \pm d\right\}$ where $\theta \in \left\{\frac{\sqrt{2}}{2}d, \frac{\sqrt{3}}{2}d, \frac{1}{2}d\right\}$ and d is even.

The following corollary shows that if G is a regular bipartite graph and squares of its eigenvalues are rational numbers, then Grover's walk defined over G is periodic with period k if and only if the bipartite walk defined over G is periodic with period τ. Moreover, by Section 4.5, we know k is even and $\tau = \frac{k}{2}$.

5.5.3 Corollary. *Let G be a regular bipartite graph. Assume that the square of each eigenvalue of G is rational. Then G is periodic if and only if $S(G)$ is periodic.*

Proof. Let λ_r be an eigenvalue of G. By Theorem 5.3.4, the graph G is periodic if and only if

$$\lambda_r^2 \in \left\{0, \frac{1}{2}d^2, \frac{3}{4}d^2, \frac{1}{4}d^2, d^2\right\}.$$

By Corollary 5.5.1, graph $S(G)$ is periodic. □

5.6 Examples and open questions

Given a graph X, the *bipartite double cover* of X is the Kronecker product $X \times K_2$. The vertex set of $X \times K_2$ is $V(X) \times V(K_2)$ and two vertices are adjacent if

(i) their first components are adjacent in X, and

(ii) their second components are adjacent in K_2.

Let $V(P_2) = \{0, 1\}$ and $V(K_2) = \{0, 1\}$. The graph shown in Figure 5.1b is the bipartite double cover of P_2.

(a) P_2 (b) Bipartite double cover of P_2

Let G denote the graph shown in Figure 5.2. The bipartite double cover of G is a 4-regular bipartite graph.

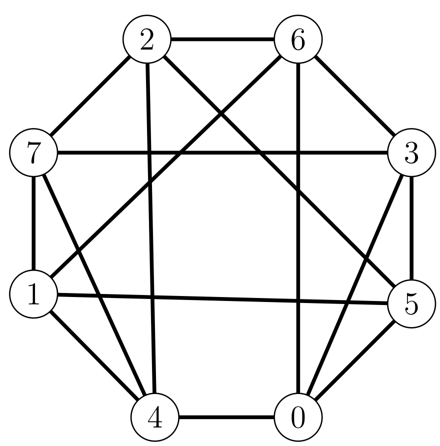


Figure 5.2: G

The adjacency matrix of G has spectrum

$$\{-(1+\sqrt{5}), -2, 0, \sqrt{5}-1, 4\}.$$

The adjacency matrix of $G \times K_2$ has spectrum

$$\{\pm(1+\sqrt{5}), \pm 2, 0, \pm(\sqrt{5}-1), \pm 4\}.$$

By Theorem 5.3.4, the bipartite walk defined over $G \times K_2$ is periodic. It has period $\tau = 10$.

By Corollary 5.5.1, the bipartite walk over the subdivision graph of $G \times K_2$ is periodic. In other words, Grover's walk defined over $G \times K_2$ is periodic. Moreover, by Corollar 4.5.2, it has period $\tau = 20$.

Another example we would like to show is $\operatorname{Cayley}(\mathbb{Z}_{10}, \{\pm 1, \pm 4\})$. It is a 4-regular graph and it has eigenvalues

$$\{-(1+\sqrt{5}), 0, \sqrt{5}-1, 4\}.$$

The bipartite double cover of $\operatorname{Cayley}(\mathbb{Z}_{10}, \{\pm 1, \pm 4\})$ has spectrum

$$\{\pm(1+\sqrt{5}), 0, \pm(\sqrt{5}-1), \pm 4\}.$$

By Theorem 5.3.4, the bipartite walk defined over the bipartite double cover of $\operatorname{Cayley}(\mathbb{Z}_{10}, \{\pm 1, \pm 4\})$ is periodic. It has period $\tau = 10$. By Corollary 5.5.1, the bipartite walk defined over the subdivision graph of $\operatorname{Cayley}(\mathbb{Z}_{10}, \{\pm 1, \pm 4\})$ is periodic with period $\tau = 20$.

Graph $G \times K_2$, its subdivision graph and the subdivision graph of $\operatorname{Cayley}(\mathbb{Z}_{10}, \{\pm 1, \pm 4\})$ are only three periodic bipartite graphs we have found such that they have eigenvalues λ with

$$\lambda^2 \in \left\{\frac{5 \pm \sqrt{5}}{8} d_0 d_1, \frac{3 \pm \sqrt{5}}{8} d_0 d_1\right\}.$$

We want to know if there are more such periodic bipartite graphs.

The characterization in Theorem 5.3.4 is nice in the sense that using the spectrum of the underlying graph alone, we can decide if the walk is periodic or not. But on the other hand, Theorem 5.3.4 still put a constraint on the spectrum of the underlying biregular graph, i.e., squares of eigenvalues are algebraic integers with degree at most two. One obvious question to ask is if we can push the degree of the eigenvalues further. The author believes Theorem 3.3 in [35] will shed some light on the question.

In continuous quantum walks, there is a complete characterization of periodic walks.

5.6.1 Theorem (Corollary 3.3 [15]). *A graph X is periodic if and only if either:*

(a) The eigenvalues of X are integers, or

(b) The eigenvalues of X are rational multiples of $\sqrt{\Delta}$, for some square-free integer Δ.

If the second alternative holds, X is bipartite. □

As stated before, in general, there is no obvious connection between a discrete quantum walk and the spectrum of the underlying graph if there is no assumption on the underlying graph at all. Although our ultimate goal is to find a complete characterization of periodic bipartite walks like the one for periodic continuous walks, there is a bigger chance for us to find a similar characterization for periodic bipartite walks on biregular graphs.

Chapter 6

Incidence structures

An *incidence structure* $(\mathcal{P}, \mathcal{B})$ consists of a set of points $\mathcal{P}$, a set of blocks $\mathcal{B}$ and an incidence relation on $\mathcal{P} \times \mathcal{B}$. A point and a block are either incident or not. If they are incident, we say the point lies in the block or the block contains the point.

If $(\mathcal{P}, \mathcal{B})$ is an incidence structure, its *incidence graph* is a bipartite graph with bipartition $(\mathcal{P}, \mathcal{B})$, where a pair of vertices u, v are adjacent if one is a point and the other is a block that contains it. An incidence structure is *thick* if the minimum valency of its incidence graph is at least three.

In this chapter, we will look into the bipartite walks of the incidence graph of two incidence structures: t-designs with $t \geq 2$ and generalized quadrangles.

The *incidence matrix* of a finite incidence structure $(\mathcal{P}, \mathcal{B})$ is the 01-matrix with rows indexed by $\mathcal{P}$, columns indexed by $\mathcal{B}$ and with $N_{x,B} = 1$ if and only if the point x is incident with the block B. Then the adjacency matrix of the incidence graph is

$$\begin{pmatrix} \mathbf{0} & N \\ N^T & \mathbf{0} \end{pmatrix}.$$

The incidence matrix is an important tool we use to study the bipartite walk defined on the incidence structure.

For bipartite walks on t-designs and bipartite walks on generalized quadrangles, we give formulas for their Hamiltonians. We introduce some graph properties of their H-(di)graphs. We show that if the underlying graph is the incidence graph of a partial linear design, then the H-digraph is exactly the distance-two graph of the line graph of the incidence graph. If the bipartite walk is defined on the incidence graph of a generalized quadrangle, we show that the transition matrix lies in a homogeneous coherent algebra, which is a powerful tool for us to study behavior of the walk.

We give a summary at the end of the chapter.

6.1 t-designs with $t \geq 2$

An incidence structure $(\mathcal{P}, \mathcal{B})$ is *point regular* if each point is incident with the same number of blocks; it is *block regular* if each block is incident with the same number of points. A *t-design* is a block-regular incidence structure such that each subset of t points is incident with exactly λ_t blocks. We denote the number of blocks that contain a given set of i points by λ_i.

Let $\mathcal{D} = (\mathcal{P}, \mathcal{B})$ be a t-design with parameters (v, b, r, k, λ_t). Then $\mathcal{D}$ satisfies that

(i) $|P| = v$ and $|\mathcal{B}| = b$,

(ii) every point is incident with r blocks,

(iii) every block contains k points,

(iv) every subset of t points are contained in exactly λ_t blocks.

A design with $v = b$ is called a *symmetric design*. Note that $b = v$ if and only if $r = k$.

A *flag* (x, B) of $\mathcal{D}$ is a point-block pair such that the point x is contained in the block B. Let G be the incidence graph of $\mathcal{D}$. Each edge of G corresponds to a flag of $\mathcal{D}$. If two flags share the same block, then we say they are in the same cell of partition π_0. Similarly, if two flags have the same point, then they are in the same cell of partition π_1. So, we have two partitions of flags of $\mathcal{D}$.

6.2 Bipartite walks on t-designs for $t \geq 2$

In this section, we define bipartite walk U on the incidence graph of a t-design $\mathcal{D}$ with $t \geq 2$. We give a formula for the Hamiltonian H of U. In this case, the Hamiltonian has a very nice form, i.e., all the non-zero entries of H are $\pm\alpha$ for some constant α and α is determined by the parameters of $\mathcal{D}$. In other words, the H-digraph has constant weight and the weight is determined by the parameters of $\mathcal{D}$, which we will prove in Section 6.4.

Let $\mathcal{D} = (\mathcal{P}, \mathcal{B})$ be a t-design with parameters (v, b, r, k, λ_t). Now we are going to define the bipartite walk on the incidence graph G of $\mathcal{D}$.

Let P_0, P_1 be the characteristic matrices of partitions π_0, π_1 respectively. Let $\widehat{P}_0$ and $\widehat{P}_1$ denote the normalized P_0 and P_1. Since G is (r, k)-biregular, we have that

$$\widehat{P}_0 = \frac{1}{\sqrt{k}} P, \quad \widehat{P}_1 = \frac{1}{\sqrt{r}} P_1.$$

Let $P = \widehat{P}_0 \widehat{P}_o^T$ and $Q = \widehat{P}_1 \widehat{P}_1^T$ and we define the transition matrix of the bipartite walk over G to be

$$U = (2P - I)(2Q - I).$$

One reason we choose to study bipartite walks on t-designs is that the Hamiltonian of the walk has a clean formula. This helps us to show that the corresponding H-digraph has constant weight on its arcs, which will be proved in Section 6.4.

6.2.1 Theorem. *Let G be the incidence graph of a t-design $\mathcal{D}$ with parameters (v, b, r, k, λ_t). Let U denote the transition matrix of the bipartite walk defined on G. Then the Hamiltonian of U is*

$$H = -\theta \frac{2i}{\sin(\theta)} (PQ - QP).$$

Proof. Let N be the incidence matrix of $\mathcal{D}$. Note that we can write

$$N = P_1^T P_0.$$

We define

$$\widehat{N} = \widehat{P}_1^T \widehat{P}_0 = \frac{1}{\sqrt{rk}} N,$$

and then we have

$$\widehat{N} \widehat{N}^T = \frac{1}{rk} N N^T.$$

As shown in Chapter 2, eigenvalues of U are determined by eigenvalues of $\widehat{N}\widehat{N}^T$. First consider the spectrum of NN^T. We have that

$$NN^T = (r - \lambda_2) I + \lambda_2 J, \tag{6.2.1}$$

where

$$\lambda_2 = \frac{\lambda_t \binom{v-2}{t-2}}{\binom{k-2}{t-2}}.$$

Combining Equation 6.2.1 with the identity

$$\frac{v-1}{k-1} = \frac{r}{\lambda_2},$$

we conclude that the eigenvalues of NN^T are $\{r - \lambda_2, rk\}$ and their corresponding idempotents are

$$E_{r-\lambda_2} = I - \frac{1}{v}J, \quad E_{rk} = \frac{1}{v}J.$$

So, the eigenvalues of $\widehat{N}\widehat{N}^T$ are

$$\left\{\frac{1}{rk}(r - \lambda_2), 1\right\}$$

and the corresponding idempotents are

$$E_1 = \frac{1}{v}J, \quad E_{\frac{r-\lambda_2}{rk}} = I - \frac{1}{v}J.$$

Following Corollary 2.2.6, we choose θ such that $\cos\theta = \frac{2(r-\lambda)}{rk} - 1$ and we set

$$W := \widehat{P}_1(I - \frac{1}{v}J)\widehat{P}_1^T.$$

Then the Hamiltonian of U is

$$\begin{aligned}
H &= \theta\left(E_\theta - \overline{E_\theta}\right) \\
&= -\theta\frac{2i}{\sin(\theta)}\left(PW - WP\right) \\
&= -\theta\frac{2i}{\sin(\theta)}\left(\widehat{P}_0\widehat{P}_0^T\widehat{P}_1(I - \frac{1}{v}J)\widehat{P}_1^T - \widehat{P}_1(I - \frac{1}{v}J)\widehat{P}_1^T\widehat{P}_0\widehat{P}_0^T\right) \\
&= -\theta\frac{2i}{\sin(\theta)}\left(PQ - QP - \frac{1}{v}P\widehat{P}_1J\widehat{P}_1^T + \frac{1}{v}\widehat{P}_1J\widehat{P}_1^TP\right).
\end{aligned}$$

Since each cell of P_1 has the same size (i.e., r), we get that

$$\widehat{P}_1J\widehat{P}_1^T = \frac{1}{r}J.$$

Since each cell of P_0 has the same size(i.e., k), we know that $PJ = JP$. Thus, we get that the Hamiltonian of U is

$$H = -\theta \frac{2i}{\sin(\theta)}(PQ - QP). \qquad \square$$

6.3 Relations between flags

One important tool we used in studying the bipartite walks over the incidence graph of t-designs is a slightly modified version of the three-class association scheme on flags proposed by Chakravarti in [7].

Let $f_1 = (x, B), f_2 = (x', B')$ be two flags of the design $\mathcal{D} = (\mathcal{P}, \mathcal{B})$, where $x, x' \in \mathcal{P}$ and $B, B' \in \mathcal{B}$. We say f_1, f_2 are 1-*associated* if either $x = x'$ or $B = B'$. Flag f_1 is $2A$-*associated* with flag f_2 if $x \neq x', B \neq B'$, and x is incident with B'. Similarly, flag f_1 is $2B$-*associated* with flag f_2 if $x \neq x', B \neq B'$, and x' is incident with B.

(a) (x, B) is $2A$-associated with (x', B') (b) (x, B) is $2B$-associated with (x', B')

We define two flags to be 2-*associated* if they are either $2A$-associated or $2B$-associated. Note that if a flag f_1 is $2A$-associated with a flag f_2, then the flag f_2 is $2B$-associated with flag f_1 and vice versa. Also, two flags can be both $2A$-associated and $2B$-associated. If two flags are neither 1-associated nor 2-associated, then they are 3-*associated*.

Given a flag $f_1 = (x, B)$ in a t-design with parameters (v, b, r, k, λ_t), we have that

(i) the number of flags that are 1-associated with f_1 is $(k-1)+(r-1)$;

(ii) the number of flags that are $2A$-associated with f_1 is $(r-\lambda_2)(k-1)$;

(iii) the number of flags that are $2B$-associated with f_1 is $(r-\lambda_2)(k-1)$.

6.4 H-digraphs and H-graphs

We study the Hamiltonian H of U when $\mathcal{D}$ is symmetric and the Hamiltonian H of U^2 when $\mathcal{D}$ is not symmetric. From now on, when we say the H-(di)graph, we refer to the (di)graph raised from the Hamiltonian of U when $\mathcal{D}$ is symmetric and the (di)graph raised from the Hamiltonian of U^2 when $\mathcal{D}$ is not symmetric.

In general, given a bipartite walk on a graph, we do not know much about the H-(di)graph that associated with it. But when we consider the bipartite walk defined over the incidence graph of a t-design, using the structure of the design, there are several things we can say about the H-(di)graph. In this section, we show that the H-digraph always has the constant weight on its arcs. We will also introduce some nice graph properties of the H-(di)graph, such as its valencies, diameter, and girth. Moreover, if $\mathcal{D}$ is symmetric, we can show that the H-graph is the distance-2 graph of the line graph of G if and only if G has girth greater than four, i.e., the design $\mathcal{D}$ is a projective plane. In other words, the incidence graph of the design determines the bipartite walk defined over it.

Let $\mathcal{D}$ be a t-design with parameters (v, b, r, k, λ_t) and its incidence matrix is N. Let G be the incidence graph of $\mathcal{D}$. Then the adjacency matrix of G is

$$A(G) = \begin{pmatrix} \mathbf{0} & N \\ N^T & \mathbf{0} \end{pmatrix}.$$

Thus, the matrix $A(G)$ is invertible if and only if N is invertible.

6.4.1 Theorem. *The incidence matrix of a symmetric t-(v, k, λ_t) design $\mathcal{D}$ is invertible.*

Proof. As shown in previous section, the matrix

$$NN^T = (r - \lambda_2)\, I + \lambda_2 J$$

has spectral decomposition

$$NN^T = (r - \lambda_2)\left(I - \frac{1}{v}J\right) + rk \cdot \frac{1}{v}J.$$

Then we have that

$$\det(NN^T) = (r - \lambda_2)^{v-1} rk.$$

Since $\lambda_2(v-1) = r(k-1)$ and $v > k$, we have that $r > \lambda_2$. Thus,

$$\det(NN^T) > 0.$$

Since $\mathcal{D}$ is symmetric (i.e. N is a square matrix),

$$\det(NN^T) = \det(N)\det(N^T) = \det(N)^2.$$

Thus, $\det(N) \neq 0$, which implies that N is invertible. □

By Theorem 2.4.2, there exists a skew-symmetric matrix S such that the Hamiltonian H can be written as

$$H = iS$$

if and only if $\mathcal{D}$ is symmetric.

When $\mathcal{D}$ is symmetric, we study the Hamiltonian of U and the corresponding H-digraph and H-graph. In the case when $\mathcal{D}$ is not symmetric, we consider the Hamiltonian H of U^2 and the corresponding H-digraph and H-graph.

Now we are going to introduce some properties of the H-(di)graph.

6.4.2 Corollary. *Let G be the incidence graph of a t-design $\mathcal{D}$ with parameters (v, b, k, r, λ_t). Consider the bipartite walk defined over G. Then the H-digraph has constant weight on its arc. If $\mathcal{D}$ is symmetric, the weight on arcs of the H-digraph is*

$$-\frac{2\theta i}{\sin(\theta) rk}$$

and if $\mathcal{D}$ is not symmetric, the weight on arcs of the H-digraph is

$$-\frac{4\theta i}{\sin(\theta) rk}.$$

Proof. From Theorem 6.2.1, we know that the Hamiltonian of U is

$$H = -\theta\frac{2i}{\sin(\theta)}(PQ - QP).$$

Using the same argument in the proof of Theorem 6.2.1, we can show that the Hamiltonian of U^2 is

$$H = -\theta\frac{4i}{\sin(\theta)}(PQ - QP).$$

For a point x and a block B, there is at most one flag f with $f = (x, B)$, following from which, we know that both PQ and QP are $\left(0, \frac{1}{rk}\right)$-matrices. Thus, the entries of $PQ - QP$ are 0 or $\pm\frac{1}{rk}$.

When $\mathcal{D}$ is symmetric, let $A(\overrightarrow{H})$ be the skew-adjacency matrix of H-digraph, then we have

$$A(\overrightarrow{H}) = rk(PQ - QP)$$

and

$$H = -\frac{2\theta i}{\sin(\theta) rk} A(\overrightarrow{H}). \tag{6.4.1}$$

So we can see that the H-digraph is an oriented graph with constant weight

$$-\frac{2\theta i}{\sin(\theta) rk}.$$

Similarly, when $\mathcal{D}$ is not symmetric, we have that the Hamiltonian of U^2 can be written as

$$H = -\frac{4\theta i}{\sin(\theta) rk} A(\overrightarrow{H}),$$

where $A(\overrightarrow{H}) = rk(PQ - QP)$. □

We can see that whether the design $\mathcal{D}$ is symmetric or not, the H-digraph has constant weight and the weight is determined by the parameters of $\mathcal{D}$.

6.4.3 Theorem. *Let G be the incidence graph of a t-design $\mathcal{D}$ with parameters (v, b, k, r, λ_t). Consider the bipartite walk defined over G. Then the H-digraph is Eulerian with*

$$\textit{in-degree}(u) = \textit{out-degree}(u) = (k-1)(r - \lambda_2)$$

for every vertex u of the H-digraph.

Proof.

The skew-symmetric adjacency matrix of the H-digraph is

$$A(\overrightarrow{H}) = rk(PQ - QP).$$

Based on the definition of P, Q, we know that

$$(PQ - QP)_{i,j} = 0$$

if and only if flags corresponding to the i-th and j-th rows are both $2A$- and $2B$-associated with each other.

As shown in the previous section, given a flag f, the number of flags that are exclusively $2A$-associated with f is

$$(k-1)(r-\lambda_2),$$

which is the same as the number of flags that are exclusively $2B$-associated with f.

The number of non-zero entries in each row of $PQ - QP$ is

$$2(k-1)(r-\lambda_2),$$

which is the degree of H-graph. Since $\mathcal{D}$ is point-regular and block-regular, we know that $\mathbf{1}$ is an eigenvector of both P and Q. It follows that $\mathbf{1}$ is an eigenvector of $PQ - QP$ with eigenvalue 0, which means that

$$\text{in-degree}(u) = \text{out-degree}(u)$$

for every vertex u of H-digraph. Thus, the H-digraph is Eulerian and it has

$$\text{in-degree}(u) = \text{out-degree}(u) = (k-1)(r-\lambda_2)$$

for every vertex u. □

The H-digraph being Eulerian makes it easy for us to assess the connectivity of the H-digraph.

6.4.4 Corollary. *Let G be the incidence graph of t-design $\mathcal{D}$. Consider the bipartite walk defined over G. The H-digraph is weakly connected if and only if it is strongly connected.*

Proof. Lemma 2.6.1 in [18] states that every weakly connected component of a Eulerian oriented graph is strongly connected. □

6.4.5 Theorem. *Let $\mathcal{D}$ be a thick t-design ($t \geq 2$) with parameters (v, b, r, k, λ_t) and its incidence graph G has girth ≥ 6. Let U be the transition matrix of the bipartite walk over G and H is the Hamiltonian of U. Then the H-graph has diameter 2.*

Proof. Since the girth of G is at least six, there is no 4-cycle, which implies that there are no two flags that are both $2A$- and $2B$-associated with each other. From the proof of Theorem 6.4.3, we know that two vertices are not adjacent in the H-graph if and only if their corresponding flags are either 1-associated or 3-associated with each other. Let $f_1 = (x_1, B_1), f_2 = (x_2, B_2)$ be two flags whose corresponding vertices are not adjacent in the H-graph. First consider the case when f_1 and f_2 are 1-associated, i.e., they share either a block or a point. If they share a point x, i.e., $x = x_1 = x_2$, then since $\mathcal{D}$ is thick, there exists $f_3 = (x, B_3)$, where $B_3 \neq B_1, B_3 \neq B_2$. Since G has girth six and degree at least three, there exists a flag $f_4 = (x_4, B_3)$ where $x_4 \neq x$. Thus, flag f_1, f_2 are both $2A$-associated with f_4. Then the corresponding vertices of $\{f_1, f_4, f_2\}$ form a path from f_1-vertex to f_2-vertex in the H-graph. A similar argument works for the case when f_1, f_2 share a block.

Now consider the case when f_1 and f_2 are 3-associated. Since $\mathcal{D}$ is a t-design and $t \geq 3$, there exists a block B such that x_1, x_2 are both contained in B. Since G has degree at least three, there exists a flag $f = (x', B)$ such that $x' \neq x_1$ and $x' \neq x_2$. Then f_1, f_2 are both $2A$-associated with f. Then the corresponding vertices of $\{f_1, f, f_2\}$ form a path from f_1-vertex to f_2-vertex in the H-graph.

Therefore, we conclude that the diameter of the H-graph is two. □

6.4.6 Theorem. *Let $\mathcal{D}$ be a t-design with $t \geq 2$. If the incidence graph G of $\mathcal{D}$ has girth $2d$ with $d \geq 3$, then the H-graph raised from the bipartite walk on G has girth d.*

Proof. Let $U = (2P - I)(2Q - I)$ be the transition matrix of the bipartite walk on G. We have shown that when $\mathcal{D}$ is symmetric, the Hamiltonian is

$$H = -\theta \frac{2i}{\sin(\theta)}(PQ - QP).$$

Since the incidence graph has girth ≥ 6, the two flags f_1, f_2 are adjacent in the H-graph if f_1, f_2 are either $2A$- or $2B$-associated with each other, but cannot be both $2A$- and $2B$-associated. So a $2d$-cycle in G corresponds to a d-cycle in the H-graph. The same argument applies when $\mathcal{D}$ is not symmetric, i.e., when H is the Hamiltonian of U^2. □

Note that both Theorem 6.4.5, 6.4.6 require that the incidence graph G has girth ≥ 6. There exists a cycle of length four in G if and only if there are two distinct flags that are both $2A$- and $2B$-associated with each other. Let LG_i denote the i-th distance matrix of the line graph of the incidence graph G of $\mathcal{D}$. Now we are going to show that if $\mathcal{D}$ is symmetric, regardless of the girth of the incidence graph of $\mathcal{D}$, the adjacency matrix of the H-graph is a polynomial in $A(LG), A(LG_2)$. Moreover, we can prove that if the design $\mathcal{D}$ is symmetric and its incidence graph has girth ≥ 6 if and only if $A(H) = A(LG_2)$.

If G has girth four, there exists a unique 4-cycle that contains both f_1, f_2 in G. This implies that there exist exactly two paths of length two from f_1-vertex to f_2-vertex in the line graph of G. Given a matrix M, we define a 01-matrix $\mathrm{Pos}(M, s)$ such that

$$(\mathrm{Pos}(M, s))_{i,j} = 1$$

if $M_{i,j} = s$. Let LG_i denote the i-th distance graph of the line graph of G. Then we have that

$$A(LG_2) - A(H) = \begin{cases} \mathrm{Pos}\left(A(LG)^2, 2\right) & \text{if } r \neq 4 \text{ and } k \neq 4; \\ \mathrm{Pos}\left(A(LG)^2, 2\right) - 4Q + I & \text{if } r = 4 \text{ and } k \neq 4; \\ \mathrm{Pos}\left(A(LG)^2, 2\right) - 4P + I & \text{if } k = 4 \text{ and } r \neq 4; \\ \mathrm{Pos}\left(A(LG)^2, 2\right) - 4P - 4Q + 2I & \text{if } r = k = 4. \end{cases} \tag{6.4.2}$$

Now we are going to write $\mathrm{Pos}\left(A(LG)^2, 2\right)$ in terms of $A(LG)$ and $A(LG_2)$. Note that $A(LG)^2_{i,j}$ is the number of paths of length two between f_i and f_j. If $r = k$, we have that

$$A(LG)^2_{i,j} = \begin{cases} 2k - 2 & \text{if } i = j; \\ k - 2 & \text{if } f_i, f_j \text{ are 1-associated (i.e., } A(LG)_{i,j} = 1); \\ 1 & \text{if } f_i, f_j \text{ are exclusively either } 2A \text{ or } 2B\text{-associated;} \\ 2 & \text{if } f_i, f_j \text{ are both } 2A \text{ and } 2B\text{-associated.} \end{cases}$$

If $r \neq k$, we have that

$$A(LG)^2_{i,j} = \begin{cases} r+k-2 & \text{if } i=j; \\ k-2 & \text{if } f_i, f_j \text{ are 1-associated and they share the same block;} \\ r-2 & \text{if } f_i, f_j \text{ are 1-associated and they share the same point;} \\ 1 & \text{if } f_i, f_j \text{ are exclusively either } 2A \text{ or } 2B\text{-associated;} \\ 2 & \text{if } f_i, f_j \text{ are both } 2A \text{ and } 2B\text{-associated.} \end{cases}$$

Therefore, if $r = k$ but $r, k \neq 4$, we have that

$$\operatorname{Pos}(A(LG)^2, 2) = A(LG)^2 - (2k-2)I - (k-2)A(LG) - A(LG_2), \quad (6.4.3)$$

and if $r = k = 4$, we have that

$$\operatorname{Pos}(A(LG)^2, 2) - 4P - 4Q + 2I = A(LG)^2 - 2I - 2A(LG) - A(LG_2). \quad (6.4.4)$$

6.4.7 Theorem. *Let $\mathcal{D}$ be a symmetric t-design with $t \geq 2$. Let LG_i denote the i-th distance matrix of the line graph of the incidence graph G of $\mathcal{D}$. Let $A(H)$ denote the adjacency matrix of the H-graph. Then*

$$A(H) \in \langle I, A(LG), A(LG_2), A(LG_3) \rangle.$$

Proof. From Equations 6.4.2, we know that if $r, k \neq 4$,

$$A(LG_2) - A(H) = \operatorname{Pos}\big(A(LG)^2, 2\big)$$

and if $r = k = 4$, we have

$$A(LG_2) - A(H) = \operatorname{Pos}\big(A(LG)^2, 2\big) - 4P - 4Q + 2I.$$

Then from Equation 6.4.3 and Equation 6.4.4, we have that if $r, k \neq 4$,

$$A(H) = A(LG_2) - A(LG)^2 + (2k-2)I + (k-2)A(LG) + A(LG_2)$$

and if $r = k = 4$,

$$A(H) = A(LG_2) - A(LG)^2 + 2I + 2A(LG) + A(LG_2). \qquad \square$$

Now we have shown that if the design $\mathcal{D}$ is symmetric, the H-graph that comes from the bipartite walk is determined by the design. If $\mathcal{D}$ is a projective plane, the H-graph is exactly the distance-2 graph of the line graph of G.

6.4.8 Theorem. *Let $\mathcal{D}$ be a symmetric t-design with $t \geq 2$ with $r, k \neq 4$ and let G be the incidence graph of $\mathcal{D}$. Then $\mathcal{D}$ is a projective plane if and only if the H-graph obtained from the bipartite walk over G is the distance-2 graph of the line graph of G.*

Proof. From Equations 6.4.2, we have that

$$A(LG_2) - A(H) = \mathrm{Pos}\left(A(LG)^2, 2\right).$$

The incidence graph of a projective plane has girth six. Based on the discussion above, the incidence graph G has no 4-cycles if and only if

$$\mathrm{Pos}(A(LG)^2, 2) = 0.$$

The theorem follow immediately. □

6.5 Behavior of the walk

In this section, we use the average mixing matrix to study the limiting behavior of the bipartite walk defined over the incidence graph of a t-design. We also show that there are no periodic states in the walk defined over the incidence graph of a t-design, which implies that there is no perfect state transfer.

Let U be the transition matrix of a bipartite walk. We define the *mixing matrix* $M_U(k)$ of U at the k-th step by

$$M_U(k) = U^k \circ U^{-k}.$$

Sometimes we omit the subscript when U is clear. The value of the entry $(M_U(k))_{i,j}$ is the probability that the system is at state e_j, given that the initial state is e_i.

One matrix that helps us understanding the behavior of the walk is the average mixing matrix. As shown by Aharonov et al. in [1], the sequence

$$\{M_U(0), M_U(1), \cdots\}$$

does not converge in general, unless U is the identity matrix. So to understand the limiting behavior of the walk, we instead study its average mixing matrix.

Given the transition matrix U of a bipartite walk, the *average mixing matrix* of U is

$$\widehat{M}_U = \lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} U^k \circ U^{-k}.$$

Using the spectral decomposition of the transition matrix, we give another definition of the average mixing matrix of the walk.

The average mixing matrix of the bipartite walk defined on the incidence graph of a symmetric design is closely related to the underlying bipartite graph and its line graph.

6.5.1 Theorem. *Let U denote the transition matrix of a bipartite walk. If U has spectral decomposition $U = \sum_r \theta_r E_r$, then the average mixing matrix of U is*

$$\widehat{M}_U = \sum_r E_r \circ \overline{E_r}.$$

Proof. The mixing matrix of U at step k is

$$\begin{aligned} M_U(k) &= U^k \circ U^{-k} \\ &= \sum_r E_r \circ \overline{E_r} + \sum_{r\neq s} \exp\left(ik(\theta_r - \theta_s)\right) E_r \circ \overline{E_s} \\ &= \sum_r E_r \circ \overline{E_r} + 2\sum_{r<s} \cos(\theta_r - \theta_s) E_r \circ \overline{E_s}, \end{aligned}$$

where we use that $\sin(x)$ is an odd function. Using that

$$\lim_{k\to\infty} \frac{1}{K} \sum_{k=0}^{K} \cos(\varphi k) = 0$$

for any non-zero φ, we have

$$\widehat{M}_U = \lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} U^k \circ U^{-k} = \sum_r E_r \circ \overline{E_r}. \qquad \square$$

6.5.2 Theorem. *Let G be the incidence graph of a symmetric t-design $\mathcal{D}$ with $t \geq 2$. Let U be the transition matrix of the bipartite walk over G. Then*

$$\widehat{M}_U \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle.$$

Proof. Write the spectral decomposition of U as

$$U = E_1 + e^{i\theta_r} E_r + e^{-i\theta_r} \overline{E_r}.$$

Let $E_r = A_r + iB_r$. The average mixing matrix of U is

$$\widehat{M_U} = E_1^{\circ 2} + 2\left(A_r^{\circ 2} + B_r^{\circ 2}\right).$$

Then the Hamiltonian of U is

$$H = \theta_r(E_r - \overline{E_r}) = 2i\theta_r B_r,$$

which implies that

$$H \circ H = -4\theta_r^2 B_r^{\circ 2} = \frac{4\theta^2}{\sin \theta^2 r^2 k^2} A(H),$$

where the last equality comes from Equation 6.4.1. Thus, we get that

$$B^{\circ 2} = \frac{-1}{\sin \theta^2 r^2 k^2} A(H).$$

From Theorem 6.4.7, we know that $A(H) \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle$, which gives us that

$$B^{\circ 2} \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle.$$

Let $A(LG) = \sum_s \lambda_s F_s$ be the spectral decomposition of $A(LG)$. As shown in Theorem 2.5.1, we have that

$$A_r = \frac{1}{2}(I - E_1) = \frac{1}{2}\left(I - (F_{-2} + F_{2(d-1)}\right).$$

Since both $F_{-2}, F_{2(d-1)}$ are polynomials in $A(LG)$,

$$A_r^{\circ 2} \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle,$$

and

$$E_1^{\circ 2} \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle.$$

Therefore, we can conclude that

$$\widehat{M_U} \in \langle I, A(LG), A(LG_2), A(LG_3)\rangle. \qquad \square$$

The theorem below shows that in the limit, the probability of the walker going back to where she started is at least $\frac{1}{3}$.

6.5.3 Theorem. *Let U be the transition matrix of the bipartite walk defined over a symmetric design $\mathcal{D}$. Then*

$$\widehat{M}_{i,i} \geq \frac{1}{3}.$$

Proof. Assume the transition matrix U has spectral decomposition

$$U = E_1 + e^{i\theta_r} E_r + e^{-i\theta_r} \overline{E_r}.$$

Let $E_r = A_r + iB_r$. The average mixing matrix of U is

$$\widehat{M} = E_1^{\circ 2} + 2\left(A_r^{\circ 2} + B_r^{\circ 2}\right).$$

Since E_r has real diagonal, we have that

$$\widehat{M}_{i,i} = (E_1)_{i,i}^2 + 2\left((A_r)_{i,i}\right)^2.$$

Using that

$$A_r = \frac{1}{2}(I - E_1),$$

we write

$$\widehat{M}_{i,i} = (E_1)_{i,i}^2 + 2\left(\frac{1}{2}(I - E_1)_{i,i}\right)^2$$

Let $(E_1)_{i,i} = x$. Then we have that

$$\widehat{M}_{i,i} = x^2 + 2\left(\frac{1}{4}(1 + x^2 - 2x)\right) = \frac{1}{2}(3x^2 - 2x + 1),$$

which reaches minimum $\frac{1}{3}$ at $x = \frac{1}{3}$. □

A quantum walk with average mixing matrix

$$\widehat{M} = \alpha J$$

for some constant α, is said to admit *uniform average mixing*. By the definition of $\widehat{M}$, uniform average mixing means that in the limit, the walker has equal chance of being on any edge, no matter which edge is the walker's initial state.

6.5.4 Corollary. *Let U be the transition matrix of the bipartite walk defined on the incidence graph of a symmetric design $\mathcal{D}$. Then $\widehat{M}_U$ does not have uniform average mixing.*

Proof. Let $\mathcal{D}$ have parameters (v, b, k, r, λ). To admit uniform average mixing, i.e., $\widehat{M}_U = \alpha J$ for some constant α, then α must equal $\frac{1}{vk} < \frac{1}{3}$. □

Theorem 6.5.3 shows that in the limit, the probability of the walker going back to where she started is at least $\frac{1}{3}$, but actually there are no periodic states.

A design is a *trivial design* if $k \in \{0, 1, v-1, v\}$.

6.5.5 Theorem. *In the bipartite walk defined over a non-trivial t-(v, k, λ_t) design with $t \geq 2$, there are no periodic states.*

Proof. Let $U = \sum_r e^{i\theta_r} E_r$ be the spectral decomposition of the transition matrix of the walk. Note that U has only two complex eigenvalues $e^{\pm i\theta}$. By Theorem 5.1.1, we know the walk has a periodic state if and only if

$$\theta \in \mathbb{Q}\pi.$$

In section 6.2, we have shown that $\cos\theta = \frac{2}{rk}(r - \lambda_2) - 1$, which is rational. Since $\cos\theta$ is a rational, by Lemma 5.3.2, we can conclude that U has a periodic state if and only if

$$\frac{2}{rk}(r - \lambda_2) - 1 = \left\{0, \pm 1, \pm\frac{1}{2}\right\}.$$

For any bipartite walk defined over a non-trivial t-design, it is not hard to see that

$$\frac{2}{rk}(r - \lambda_2) - 1 \neq 0 \text{ or } \pm 1.$$

So, the walk has a periodic state if and only if

$$\frac{2}{rk}(r - \lambda_2) - 1 = \pm\frac{1}{2}.$$

If $\frac{2}{rk}(r - \lambda_2) - 1 = \frac{1}{2}$, then it implies

$$3rk = 4(r - \lambda_2). \tag{6.5.1}$$

We know that

$$\frac{v-1}{k-1} = \frac{r}{\lambda_2}, \tag{6.5.2}$$

which implies that

$$rk = \lambda_2(v-1) + r. \tag{6.5.3}$$

Combining Equation 6.5.3 and Equation 6.5.1, we get that

$$r = \lambda_2(3v + 1),$$

which is not possible.

Similarly, combining $\frac{2}{rk}(r - \lambda_2) - 1 = \frac{1}{2}$ with Equation 6.5.2, we have that

$$3r = \lambda_2(v + 3).$$

Since $r > \lambda_2$, we must have $v + 3 < 3$, which is impossible.

Therefore, we conclude that there are no periodic states in bipartite walks defined over any non-trivial t-design with $t \geq 2$. $\square$

6.6 Projective planes

One example of bipartite walk on t-design is the bipartite walk defined on the incidene graph of a projective plane. A *projective plane* is a point-line incidence structure such that:

(a) any two distinct points lie on exactly one line,

(b) any two distinct lines have exactly one point in common,

(c) There is a set of four points such that no three are collinear.

A projective plane of order n is a 2-$(n^2 + n + 1, n + 1, 1)$ design.

Let G be the incidence graph of a projective plane of order n. Let U be the transition matrix of the bipartite walk defined on G and let H be the Hamiltonian of U. We know that the skew-adjacency matrix of H-digraph of a projective plane of order n is

$$A(\overrightarrow{H}) = (n + 1)^2 \left(PQ - QP\right).$$

From Theorem 6.4.3, 6.4.5, 6.4.6, 6.4.8, we know that

(i) The H-graph has diameter two and girth three;

(ii) The H-digraph is Eulerian with

$$\text{in-degree}(v) = \text{out-degree}(v) = n^2$$

for every vertex v;

(iii) The H-graph is the distance-2 graph of the line graph of the incidence graph.

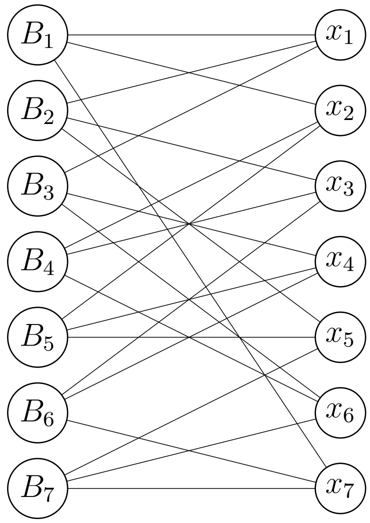


Figure 6.2: Incidence Graph of 2-$(7, 3, 1)$ design

Since the incidence graph of a projective plane of order n has girth six, that two flags are 2-associated is equivalent to them being either exclusively $2A$- or exclusively $2B$-associated with the other. Using the discussion in Section 6.2, if follows that

(i) if two flags u, v are adjacent in the H-graph, they are 2-associated;

(ii) if two flags u, v are not adjacent in the H-graph, they are either 1-associated or 3-associated.

From Section 6.3, we know that the H-graph obtained from the bipartite walk on a projective plane of order n satisfies the following:

(i) any two adjacent vertices have n common neighbours in the H-graph;

(ii) for any two non-adjacent vertices u, v in the H-graph,

  a) if u, v are 1-associated, then they have $n(n-1)$ common neighbours,

  b) otherwise they have $4(n-1)$ common neighbours.

When the underlying graph is the incidence graph of a projective plane, another way to get the results about the number of common neighbours of pairs of vertices in the H-graph shown above is using the intersection matrices presented in Section 2 in [7] by Chakaravarti. He introduces a three-class association scheme on the flags of a finite projective plane. The flag relations we introduce in Section 6.3 is a refined version of the three-class association scheme in [7]. According to the intersection matrices presented in Section 2 in [7], we know that if u, v are 2-associated, the number of flags that are 2-associated to both u, v is $p^2_{2,2} = n$. Similarly, if u, v are 1-associated, the number of flags that are 2-associated to both u, v is $p^1_{2,2} = n(n-1)$. If u, v are 3-associated, the number of flags that are 2-associated to both u, v is $p^3_{2,2} = 4(n-1)$. This agrees with the results we showed above.

Let $A_0 = I$ and define A_1 to be the adjacency matrix of the H-graph. For $k \in \{0, 1, 2, 3\}$, we define each 01-matrix A_k such that its rows and columns of are indexed by vertices of the H-graph and

$$(A_k)_{i,j} = 1$$

if v_i, v_j are k-associated.

6.6.1 Theorem. *Consider the H-graph Γ obtained from the bipartite walk on the projective plane of order n. Let $\mathcal{A} = \{A_0, A_1, A_2, A_3\}$ be a set of matrices defined as above. Then $\mathcal{A}$ forms a symmetric association scheme.*

Proof. It is easy to see that

$$\sum_{i=0}^{3} A_i = J.$$

For $m, n \in \{1, 2, 3\}$, the (i, j)-th entry of $A_m A_n$,

$$A_m A_n(i, j),$$

is the number of vertex v satisfying that

(i) v is m-associated with i and

(ii) v is n-associated with j.

From the intersection matrices presented in [7, Section 2], we know that

$$A_1 A_2(i, j) = \begin{cases} n \quad \text{if } i, j \text{ are 1-associated,} \\ n-1 \quad \text{if } i, j \text{ are 2-associated,} \\ 2 \quad \text{if } i, j \text{ are 3-associated,} \end{cases}$$

and hence, we have that

$$A_1A_2 = nA_1 + (n-1)A_2 + 2A_3.$$

Similarly, we have that

$$A_1A_3(i,j) = \begin{cases} 0 & \text{if } i,j \text{ are 1-assocaited,} \\ n & \text{if } i,j \text{ are 2-associated,} \\ 2(n-1) & \text{if } i,j \text{ are 3-associated,} \end{cases}$$

and

$$A_2A_3(i,j) = \begin{cases} n^2 & \text{if } i,j \text{ are 1-associated,} \\ 2n(n-1) & \text{if } i,j \text{ are 2-associated,} \\ 2(n-1)^2 & \text{if } i,j \text{ are 3-associated,} \end{cases}$$

which implies that

$$\begin{aligned} A_1A_3 &= nA_2 + 2(n-1)A_3, \\ A_2A_3 &= n^2A_1 + 2n(n-1)A_2 + 2(n-1)^2A3. \end{aligned}$$

The k-association is symmetric relation for each $k \in \{1,2,3\}$ and hence, matrices A_1A_2, A_2A_3, A_1A_3 are symmetric, which implies that A_1, A_2, A_3 commutes with each other and we have that

$$A_iA_j = A_jA_i \in \text{span}(\mathcal{A}).$$

Therefore, the set $\mathcal{A}$ forms a symmetric association scheme. □

Let U be the transition matrix of a discrete quantum walk, then the *mixing matrix* of the walk at step k is

$$M_U(k) = U^k \circ \overline{U^k}.$$

A sequence of discrete quantum walks, determined by transition matrices $\{U_1, U_2, \cdots\}$, is *sedentary* if

$$\lim_{n\to\infty} M_{U_n}(k) = I$$

for any step k. We are going to show that the bipartite walks on the incidence graphs of projective plane of order n form a sedentary family.

Let U be the transition matrix of the bipartite walk on the incidence graph of a symmetric t-(v, k, λ_t) design with $t \geq 2$. We consider the diagonal entries of the mixing matrix $M_U(k)$. As we have shown in Section 6.2, we have that

$$U = E_1 + e^{i\theta} E_\theta + e^{-i\theta} E_{-\theta}.$$

Following Corollary 2.2.6 , we have that

$$E_\theta = \frac{1}{\sin^2(\theta)} \left((\cos\theta + 1)W - (e^{i\theta} + 1)PW - (e^{-i\theta} + 1)WP + 2PWP \right).$$

In Section 6.2, we have shown that

$$W = \hat{P}_1 (I - \frac{1}{v} J) \hat{P}_1^T$$

So, the diagonal entry of E_θ is

$$(E_\theta)_{i,i} = \left(\frac{1}{\sin^2(\theta)} \left((\cos +1)(W - PW - WP) + 2PWP \right) \right)_{i,i}.$$

Since each cell of π_1 has size r, we have the following equations:

$$\begin{aligned} W &= Q - \frac{1}{vr} J, \\ PW &= PQ - \frac{1}{vr} PJ = PQ - \frac{1}{vr} J, \\ WP &= QP - \frac{1}{vr} PJ = QP - \frac{1}{vr} J, \\ PWP &= PQP - \frac{1}{vr} J. \end{aligned}$$

Based on how we define P, Q, it is easy to see that for all i,

$$P_{i,i} = \frac{1}{k}, \quad Q_{i,i} = \frac{1}{r},$$

and

$$(PQ)_{i,i} = (QP)_{i,i} = \frac{1}{rk}.$$

The non-zero entries of QPe_i are indexed by the flags that are either 1-associated or $2A$-associated with flag f_i, so we get that

$$(PQP)_{i,i} = e_i^T P \cdot QPe_i = k \cdot \left(\frac{1}{k} \frac{1}{rk} \right) = \frac{1}{rk}.$$

Thus, the diagonal of E_θ is constant with diagonal entry

$$\frac{1}{\sin^2(\theta)}\left((\cos\theta+1)\left(\frac{kv+k-2v}{krv}\right)+\frac{2(v-k)}{krv}\right). \tag{6.6.1}$$

Since E_1 is an idempotent, Theorem 2.2.2 gives us that

$$\operatorname{tr}(E_1)=\operatorname{rk}(E_1)=vr-v-b+2.$$

Since $E_1+E_\theta+E_{-\theta}=I$ and $E_\theta, E_{-\theta}$ have constant diagonals, we have that E_1 has constant diagonal with value

$$(E_1)_{i,i}=1-\frac{2}{r}+\frac{2}{vr}, \tag{6.6.2}$$

and hence, we can also have that

$$(E_\theta)_{i,i}=(E_{-\theta})_{i,i}=\frac{1}{r}-\frac{1}{vr}. \tag{6.6.3}$$

Let $(E_\theta)_{i,i}=\alpha$. We can write a formula for the diagonal entry of the mixing matrix at step k:

$$(M_U(k))_{i,i}=\alpha^2+(1-2\alpha)^2+4\cos(k\theta)\alpha(1-2\alpha)+2\cos(2k\theta)\alpha^2. \tag{6.6.4}$$

6.6.2 Theorem. *Let U_n denote the transition matrix of the bipartite walk defined on the incidence graph of a projective plane of order n. The bipartite walks determined by*

$$\{U_n : n\geq 2 \text{ is an integer}\}$$

form a sedentary family.

Proof. A projective plane of order n, which is a symmetric 2-$(n^2+n+1, n+1, 1)$ design. Thus, using Equation 6.6.3, the diagonal entries of E_θ are

$$\frac{n}{n^2+n+1}$$

and by Equation 6.6.2, we have

$$(E_1)_{i,i}=1-\frac{2}{r}+\frac{2}{vr}=\frac{n^2-n+1}{n^2+n+1}.$$

Using Equation 6.6.4, the diagonal entry of $\widehat{M}_{U_n}(k)$ is

$$2\left(\frac{n}{n^2+n+1}\right)^2+\left(1-\frac{2n}{n^2+n+1}\right)^2+4\cos(k\theta)\frac{n}{n^2+n+1}(1-2\frac{n}{n^2+n+1})$$
$$+2\cos(2k\theta)\left(\frac{n}{n^2+n+1}\right)^2.$$

Since

$$\lim_{n\to\infty}\frac{n}{n^2+n+1}=0,$$

we have that for any k,

$$\lim_{n\to\infty}\left(M_{U_n}(k)\right)_{i,i}=1$$

for all i, which is equivalent to that

$$\lim_{n\to\infty}M_{U_n}(k)=I. \qquad \square$$

Note that there are other sedentary families that can be obtained by bipartite walks. Let U_s denote the transition matrix of the bipartite walk defined on the incidence graph of a regular generalized quadrangle of order (s,s). The bipartite walks determined by

$$\{U_s : s\geq 1 \text{ is an integer}\}$$

also form a sedentary family. We prove this using the same idea shown in the proof of Theorem 6.6.2, so we omit the proof here. We will discuss bipartite walks defined on incidence graphs of generalized quadrangles in details in the next section.

We will end this section with a remark. One question one might ask is that if bipartite walks on two distinct projective planes of the same order behave the same. The answer is yes.

Given two non-isomorphic projective planes of the same order $\mathcal{P}_1,\mathcal{P}_2$, let G_1,G_2 denote the incidence graphs of $\mathcal{P}_1,\mathcal{P}_2$ respectively. The Whitney graph isomorphism theorem [2] states that except for K_3 and $K_{1,3}$, two connected graphs are isomorphic if and only if their line graphs are isomorphic. By Theorem 6.4.8, we can conclude that the H-graph of bipartite walk on G_1 and that of bipartite walk on G_2 are not isomorphic. That is how we can use bipartite walks to distinguish two non-isomorphic projective planes of the same order.

6.7 Generalized quadrangles

We have seen that the structure of a t-design with $t \geq 2$ actually helps us to have a nice formula for the Hamiltonian of the bipartite walk and we can use the structure of the design to get a lot of information of the H-(di)graph associated with the walk. Another incidence structure we study is generalized quadrangle, which is a 1-design.

In this section, we define a bipartite walk over the incidence graph of a generalized quadrangle and we also get a nice formula for the Hamiltonian.

We use $GQ(s,t)$ to denote a generalized quadrangle with $s+1$ points on each line and $t+1$ lines on each point. A *generalized quadrangle* $GQ(s,t)$ is a 1-(v,k,λ) design,with $k = s+1, r = t+1$ such that

(a) any two points are on the at most one line (and hence, any two lines meet in at most one point),

(b) given any line L and a point p not on L there is a unique point p' on L such that p and p' are collinear, and

(c) there are noncollinear points and nonconcurrent lines.

An incidence structure is a *partial linear space* if and only if its incidence graph has girth at least six.

For our purpose, we define a generalized quadrangle to be a partial linear space that contains noncollinear points and nonconcurrent lines, whose incidence graph has diameter four and girth eight.

Using the same way described in Section 6.2, we have two partitions of flags of $GQ(s,t)$ and following the same notations, the transition matrix of the bipartite walk defined over the incidence graph of $GQ(s,t)$ is

$$U = (2P - I)(2Q - I).$$

Similarly, we use the incidence matrix N of $GQ(s,t)$ to find a formula for the Hamiltonian of U.

The *collinearity graph* (or *point graph*) of a generalized quadrangle is a graph whose vertices are the points of the generalized quadrangle and two points are adjacent if and only if there exists a line that contains them both. Let N denote the incidence matrix of $GQ(s,t)$. The adjacency matrix of the collinearity graph of $GQ(s,t)$ is

$$NN^T - (t+1)I.$$

The incidence matrix N satisfies that

$$N\mathbf{1} = (t+1)\mathbf{1}, \quad N^T\mathbf{1} = (s+1)\mathbf{1}, \quad NN^TN = (s+t)N + J,$$

which implies that

$$(NN^T)^2 = (s+t)NN^T + (t+1)J.$$

So, the collinearity graph of a $GQ(s,t)$ is a strongly regular graph with parameters $\big((s+1)(st+1), s(t+1), s-1, t+1\big)$. The eigenvalues of the collinearity graph of a $GQ(s,t)$ are

$$\{k = s(t+1), \theta = s-1, \tau = -(t+1)\}.$$

Hence, the eigenvalues of NN^T are

$$\{k' = (s+1)(t+1), \theta' = s+t, \tau' = 0\}$$

with corresponding eigenmatrices being

$$\begin{aligned}
E_{k'} &= \frac{1}{(s+1)(st+1)}J,\\
E_{\theta'} &= \frac{m_\theta}{(s+1)(st+1)}\left(I + \frac{\theta}{k}A - \frac{\theta+1}{n-k-1}\overline{A}\right),\\
E_{\tau'} &= \frac{m_\tau}{(s+1)(st+1)}\left(I + \frac{\tau}{k}A - \frac{\tau+1}{n-k-1}\overline{A}\right),
\end{aligned}$$

where

$$A = NN^T - (t+1)I, \quad \bar{A} = J - NN^T + tI.$$

The incidence graph of $GQ(s,t)$ has degree $(s+1, t+1)$. We define

$$\widehat{N} = \frac{1}{\sqrt{(s+1)(t+1)}}N$$

and then we have

$$\widehat{N}\widehat{N}^T = \frac{1}{(s+1)(t+1)}NN^T.$$

So the eigenvalues of $\widehat{N}\widehat{N}^T$ are

$$\left\{1, \frac{s+t}{(s+1)(t+1)}, 0\right\}$$

with corresponding

$$\begin{aligned}
E_{k'} &= \frac{1}{(s+1)(st+1)} J, \\
E_{\theta'} &= \frac{(st+1)NN^T - (t+1)J}{(s+t)(st+1)} \\
E_{\tau'} &= \frac{J - (s+1)NN^T + (s^2+st+s+t)I}{(s+t)(s+1)}
\end{aligned}$$

Since N is not invertible, the adjacency matrix $A(G)$ is not invertible. Following the convention, here we let H be the Hamiltonian of $U^2 = \sum_r e^{2i\theta_r} E_r$.

Note we can write

$$E_{\theta'} = \frac{(s+1)(t+1)}{(s+t)} \widehat{N}^T \widehat{N} + \frac{(t+1)(st+1-(t+1)^2)}{(s+t)^2(st+1)} J.$$

Now following Corollary 2.2.6, we set

$$W := \hat{P}_1 E_{\theta'} \hat{P}_1^{\,T}.$$

Using that

$$\hat{P}_1 J \hat{P}_1^{\,T} = \frac{1}{t+1} J, \quad \hat{P}_1 NN^T \hat{P}_1^{\,T} = (s+1)(t+1) QPQ,$$

we have that

$$W = \frac{(s+1)(t+1)}{s+t} QPQ - \frac{1}{(s+t)(st+1)} J.$$

Let $\cos\theta = 2\theta' - 1 = 2(s+t) - 1$. Then the Hamiltonian of U^2 is

$$\begin{aligned}
H &= -i \ln(e^{2i\theta_r})(E_r - \overline{E_r}) \\
&= \theta \left(-\frac{4i}{\sin\theta} (PW - WP) \right) \\
&= -\frac{4\theta i}{\sin\theta} \cdot \frac{(s+1)(t+1)}{s+t} \left(PQPQ - QPQP \right). \qquad (6.7.1)
\end{aligned}$$

6.8 Coherent algebra $\langle P, Q\rangle$

A *coherent algebra* is a matrix algebra over $\mathbb{C}$ that is Schur-closed, closed under transpose and complex conjugation, and contains I and J. Every coherent algebra has a unique basis of 01-matrices $\mathcal{A} = \{A_0, \cdots, A_d\}$ such that

(i) $\sum_i A_i = J$,

(ii) some subset of $\mathcal{A}$ sums to I,

(iii) $A_i \circ A_j = \delta_{i,j} A_i$,

(iv) there are scalars $p_{i,j}(k)$ such that $A_i A_j = \sum_r p_{i,j}^{(r)} A_r$,

(v) $A_i^T \in \mathcal{A}$ for each i,

(vi) all non-zero rows and columns of A_i have the same sum.

A coherent algebra is *homogeneous* if I belongs to its basis.

Let P, Q be the orthogonal projections we get from the bipartite walk on the incidence graph of $GQ(s,t)$. Consider the algebra $\langle P, Q\rangle$. In this section, we show that $\langle P, Q\rangle$ is a homogeneous coherent algebra. We find the unique mutually orthogonal (with respect to Schur multiplication) basis of 01-matrices of $\langle P, Q\rangle$ and each matrix in the basis corresponds to a combinatorial relation between flags. We will also show that $U, H, A(H), A(\overrightarrow{H})$ are all contained in the coherent algebra $\langle P, Q\rangle$, which gives us another tool to analyze the walk.

For $i \in \{1, 2, \cdots, 8\}$, we define each M_i as follows. Define $M_1 = I$. The matrix

$$(M_2)_{i,j} = 1$$

if and only if two distinct flags f_i, f_j share the same block and similarly $(M_3)_{i,j} = 1$ if and only if two distinct flags f_i, f_j share the same point. Define M_4, M_5 to be matrices such that

$$(M_4)_{i,j} = 1$$

if and only if flag f_i is $2B$-associated with flag f_j and $(M_5)_{i,j} = 1$ if and only if flag f_i is $2A$-associated with flag f_j. Also, we define

$$(M_6)_{i,j} = 1$$

if and only if flag $f_j = (x_j, B_j)$ shares the same block as a flag that flag $f_i = (x_i, B_i)$ is $2B$-associated with. Similarly, $(M_7)_{i,j} = 1$ if and only if flag $f_j = (x_j, B_j)$ shares the same point as a flag that flag $f_i = (x_i, B_i)$ is $2A$-associated with.

(a) $(M_6)_{i,j} = 1$ (b) $(M_7)_{i,j} = 1$

Define

$$M_8 = J - \sum_{i=1}^{7} M_i.$$

6.8.1 Theorem. *Let P, Q be orthogonal projections that come from the bipartite walk over the incidence graph of $GQ(s,t)$. Then $\langle P, Q\rangle$ is a homogeneous coherent algebra and*

$$\{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}$$

is the unique mutually orthogonal (with respect to Schur multiplication) basis of $\langle P, Q\rangle$ that consists of 01-matrices.

Proof. First we show that $\langle P, Q\rangle$ is a coherent algebra. Using the definition of P, Q, we have the following:

$$P \circ Q = \frac{1}{(s+1)(t+1)} I,$$

$$PQPQ = \frac{s+t}{(s+1)(t+1)} PQ + \frac{1}{((s+1)(t+1))^2} J \tag{6.8.1}$$

and

$$QPQP = (PQPQ)^T = \frac{s+t}{(s+1)(t+1)} QP + \frac{1}{((s+1)(t+1))^2} J. \tag{6.8.2}$$

The algebra $\langle P, Q\rangle$ is closed under multiplication by definition and from the equations above, we know that $\langle P, Q\rangle$ contains I, J. To show that $\langle P, Q\rangle$ is a coherent algebra, we only need to show that it is closed under Schur multiplication. Since P, Q are projections, i.e.,

$$P^2 = P, \quad Q^2 = Q,$$

and Equation 6.8.1, 6.8.2, it is sufficient to show that $\{P, Q, PQ, QP, PQP, QPQ\}$ are closed under Schur multiplication.

Using the definition of P, Q and the structure of generalized quadrangles, we have the following identities.

$$PQ \circ P = QP \circ P = \frac{1}{(s+1)(t+1)}P,$$
$$PQ \circ Q = QP \circ Q = \frac{1}{(s+1)(t+1)}Q,$$

$$PQ \circ QP = \frac{1}{(s+1)^2(t+1)^2}\big((s+1)P + (t+1)Q - I\big) = QP \circ PQ,$$

$$PQP \circ P = \frac{1}{(s+1)(t+1)}P,$$

$$PQP \circ Q = \frac{1}{(s+1)(t+1)^2}I + \frac{1}{(s+1)^2(t+1)}\left(Q - \frac{1}{t+1}I\right),$$

$$QPQ \circ Q = \frac{1}{(s+1)(t+1)}Q,$$

$$QPQ \circ P = \frac{1}{(s+1)(t+1)^2}\left(P - \frac{1}{s+1}I\right) + \frac{1}{(s+1)^2(t+1)}I,$$

$$PQP \circ PQ = \frac{1}{(s+1)^2(t+1)}PQ + \left(\frac{1}{(s+1)(t+1)^2} - \frac{1}{(s+1)^2(t+1)^2}\right)P = (QPQ \circ QP)^T,$$

$$PQP \circ QP = \frac{1}{(s+1)^2(t+1)}QP + \left(\frac{1}{(s+1)(t+1)^2} - \frac{1}{(s+1)^2(t+1)^2}\right)P = (QPQ \circ PQ)^T,$$

$$\begin{aligned} PQP \circ QPQ = &\left(\frac{1}{(s+1)^2(t+1)^2} - \frac{1}{(s+1)^3(t+1)^2} - \frac{1}{(s+1)^2(t+1)^3} + \frac{2}{(s+1)^3(t+1)^3}\right) I \\ &+ \frac{1}{(s+1)^2(t+1)^2}(PQ+QP) \\ &+ \left(\frac{1}{(s+1)^3(t+1)} - \frac{2}{(s+1)^3(t+1)^2}\right) Q \\ &+ \left(\frac{1}{(s+1)(t+1)^3} - \frac{2}{(s+1)^2(t+1)^3}\right) P. \end{aligned}$$

Therefore, we can conclude that $\langle P, Q\rangle$ is indeed a coherent algebra.

Define

$$\mathcal{M} = \{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}.$$

We are going to show that $\mathcal{M}$ is the unique mutually orthogonal (with respect to Schur multiplication) basis that consists of 01-matrices of $\langle P, Q\rangle$.

It is easy to check that

$$\sum_{i=1}^{8} M_i = J, \quad M_i \circ M_j = \delta_{i,j} M_i.$$

For $i = \{1, 2, 3, 6, 7, 8\}$, the relation between flag f_i, f_j is symmetric and hence,

$$M_i = M_i^T.$$

Note that flag f_i is $2A$-associated with flag f_j if and only if flag f_j is $2B$-associated with flag f_i, which implies that

$$M_4^T = M_5.$$

Thus, the set $\mathcal{M}$ is closed under transpose. For $i \in \{1, 2, \cdots, 8\}$, using the flag relation each M_i corresponds to, we can get the following identities.

$$
\begin{aligned}
&M_2M_1 = M_2 && M_3M_1 = M_3\\
&M_2M_2 = (s-1)M_2 + sI && M_3M_2 = (M_2M_3)^T = M_5\\
&M_2M_3 = M_4 && M_3M_3 = (t-1)M_3 + tI\\
&M_2M_4 = sM_3 + (s-1)M_4 && M_3M_4 = M_7\\
&M_2M_5 = M_6 && M_3M_5 = tM_2 + (t-1)M_5\\
&M_2M_6 = sM_5 + (s-1)M_6 && M_3M_6 = M_8\\
&M_2M_7 = M_8 && M_3M_7 = tM_4 + (t-1)M_7\\
&M_2M_8 = sM_7 + (s-1)M_8 && M_3M_8 = tM_6 + (t-1)M_8
\end{aligned}
$$

$$
\begin{aligned}
&M_4M_1 = M_4 && M_5M_1 = M_5\\
&M_4M_2 = M_6 && M_5M_2 = (M_2M_4)^T\\
&M_4M_3 = tM_2 + (t-1)M_4 && M_5M_3 = (M_3M_4)^T = M_7\\
&M_4M_4 = M_8 && M_5M_4 = stM_1 + s(t-1)M_3 + (s-1)M_7\\
&M_4M_5 = stM_1 + t(s-1)M_2 + (t-1)M_6 && M_5M_5 = M_8\\
&M_4M_6 = M_2M_8 && M_5M_6 = stM_2 + s(t-1)M_5 + (s-1)M_8\\
&M_4M_7 = stM_3 + (s-1)tM_4 + (t-1)M_8 && M_5M_7 = (M_7M_4)^T = (M_3M_4M_4)^T = (M_3M_8)^T\\
&M_4M_8 = stJ - M_4\left(\sum_{i=1}^{7} M_i\right) && M_5M_8 = stJ - M_5\left(\sum_{i=1}^{7} M_i\right)
\end{aligned}
$$

$$
\begin{aligned}
&M_6M_1 = M_6 && M_7M_1 = M_7\\
&M_6M_2 = (M_2M_6)^T && M_7M_2 = (M_2M_7)^T\\
&M_6M_3 = (M_3M_6)^T && M_7M_3 = (M_3M_7)^T\\
&M_6M_4 = (M_5M_6)^T && M_7M_4 = (M_5M_7)^T\\
&M_6M_5 = (M_4M_6)^T && M_7M_5 = (M_4M_7)^T\\
&M_6M_6 = sM_4M_5 + (s-1)M_6M_5 && M_7M_6 = (M_6M_7)^T\\
&M_6M_7 = tM_2M_6 + (t-1)M_2M_8 && M_7M_7 = tM_5M_4 + (t-1)M_7M_4,\\
&M_6M_8 = s^2tJ - M_6\left(\sum_{i=1}^{7} M_i\right) && M_7M_8 = st^2J - M_7\left(\sum_{i=1}^{7} M_i\right).
\end{aligned}
$$

For $i \in \{1,2,3,6,7\}$, we have that $M_8 M_i = (M_i M_8)^T$ and $M_8 M_4 = (M_5 M_8)^T$ and $M_8 M_5 = (M_4 M_8)^T$ and

$$M_8 M_8 = s^2 t^2 J - M_8 \left(\sum_{i=1}^{7} M_i \right).$$

Thus, we can conclude that for $i, j, r \in \{1, 2, \cdots, 8\}$, there is a scalar $p_{i,j}(r)$ such that

$$M_i M_j = \sum_{r=1}^{8} p_{i,j}(r) M_r.$$

Using the structure of generalized quadrangles, we have that

$$\begin{array}{llll} M_1 J = J & M_2 J = sJ & M_3 J = tJ & M_4 J = stJ \\ M_5 J = stJ & M_6 J = s^2 tJ & M_7 J = st^2 J & M_8 J = \alpha J, \end{array}$$

where $\alpha = (st+1)(t+1)(s+1) - 1 - s - t - 2st - s^2 t - st^2$. So, every non-zero rows and columns of $M_i \in \mathcal{M}$ have the same sum. Based on how we define M_2, M_3, it is easy to see that

$$P = \frac{1}{s+1}(M_1 + M_2), \quad Q = \frac{1}{t+1}(M_1 + M_3).$$

Therefore, the set

$$\mathcal{M} = \{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}$$

indeed is the unique mutually orthogonal (with respect to Schur multiplication) basis of $\langle P, Q\rangle$ that consists of 01-matrices. □

We have shown that $\langle P, Q\rangle$ is a coherent algebra and $\mathcal{M}$ is a basis of $\langle P, Q\rangle$. Now we can write

$$\begin{aligned} U &= (2P - I)(2Q - I) \\ &= \frac{(s-1)(t-1)}{(s+1)(t+1)} M_1 - \frac{2(t-1)}{(s+1)(t+1)} M_2 - \frac{2(s-1)}{(s+1)(t+1)} M_3 + \frac{4}{(s+1)(t+1)} M_4. \end{aligned} \tag{6.8.3}$$

Using Equation 6.7.1, 6.8.1, 6.8.2, we can write the Hamiltonian of U^2 as

$$H = -\frac{4\theta i}{\sin\theta}(PQ - QP)$$

and hence, we can write

$$H = -\frac{4\theta i}{\sin\theta} \cdot \frac{1}{(s+1)(t+1)} \left(M_4 - M_5\right).$$

It follows immediately that the H-digraph has constant weight

$$-\frac{4\theta i}{\sin\theta} \cdot \frac{1}{(s+1)(t+1)}.$$

The skew-adjacency matrix of the H-digraph is

$$A(\overrightarrow{H}) = M_4 - M_5$$

and the adjacency matrix of the underlying undirected H-graph is

$$A(H) = M_4 + M_5.$$

Therefore, we can see that

$$U, H, A(\overrightarrow{H}), A(H) \in \langle P, Q\rangle.$$

6.9 Association schemes

An *association scheme* with d classes is a set $\mathcal{A} = \{A_0, \cdots, A_d\}$ of 01-matrices such that

(a) $A_0 = I$,

(b) $\sum_{i=0}^{d} A_i = J$,

(c) $A^T \in \mathcal{A}$ for each i,

(d) $A_iA_j = A_jA_i \in \operatorname{span}(\mathcal{A})$.

The *Bose-Mesner algebra* of an association scheme $\mathcal{A} = \{A_0, \cdots, A_d\}$ is the algebra generated by the matrices $A_0, \cdots, A_d$; equivalently it is the complex span of these matrices. It is a commutative algebra closed under Schur multiplication, complex conjugation and transpose. Any commutative coherent algebra is the Bose-Mesner algebra of an association scheme.

We have shown that

$$\mathcal{M} = \{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}$$

is the unique mutually orthogonal (with respect to Schur multiplication) basis of the coherent algebra $\langle P, Q \rangle$ that consist of 01-matrices. But since $\mathcal{M}$ is not necessarily commutative, the set $\mathcal{M}$ does not necessarily form an association scheme. But we are going to show that when $s = t$, there is an association scheme contained in $\langle P, Q \rangle$.

Consider the matrices

$$A_0 = M_1, \quad A_1 = M_2 + M_3, \quad A_2 = M_4 + M_5, \quad A_3 = M_6 + M_7, \quad A_4 = M_8.$$

Now we show that

$$\mathcal{A} = \{A_0, A_1, A_2, A_3, A_4\}$$

forms an association scheme.

A generalized quadrangle is a special case of a generalized d-gon with $d = 4$. A *generalized d-gon* is a point-line incidence structure whose incidence graph has diameter d and girth $2d$. It is of order (s, t) if every line contains $s + 1$ points, and every point is on $t + 1$ lines.

The following two lemmas are the standard results from algebraic graph theory.

6.9.1 Lemma. *Both the incidence graph of a regular generalized d-gon and its line graph are distance-regular.* □

6.9.2 Lemma. *The line graph of the incidence graph of a generalized d-gon has diameter d.* □

Using the two lemmas stated above, we can show that if $s = t$, there is a Bose-Mesner algebra embedded in the coherent algebra $\langle P, Q \rangle$.

6.9.3 Theorem. *Let P, Q be orthogonal projections that comes from the bipartite walk over the incidence graph of $GQ(s, s)$. Let*

$$\{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}$$

be the unique mutually orthogonal (with respect to Schur multiplication) basis of $\langle P, Q \rangle$ that consists of 01-matrices. Define

$$A_0 = M_1, \quad A_1 = M_2 + M_3, \quad A_2 = M_4 + M_5, \quad A_3 = M_6 + M_7, \quad A_4 = M_8.$$

The set $\{A_0, A_1, A_2, A_3, A_4\}$ forms an association scheme.

Proof. Let G denote the line graph of the incidence graph of a regular generalized quadrangle. By Lemma 6.9.1, 6.9.2, we know that G is a distance-regular graph with diameter four. Based on how we define M_i for $i \in \{1, 2, \cdots, 8\}$, it is not hard to see that A_r is the r-th distance matrix of G. The theorem follows. □

6.10 Bipartite walks on $GQ(s, t)$

Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix of the bipartite walk on the incidence graph of $GQ(s, t)$. Two states e_i, e_j are *cospectral* if it holds for all eigenvalue θ_r that

$$(E_r)_{i,i} = (E_r)_{j,j}\,.$$

In this section, we are going to look into some behavior of the bipartite walk defined over the incidence graph of $GQ(s, t)$. Like t-designs with $t \geq 2$, there are not strongly cospectral pairs in the walk, but here all the states are cospectral to each other. We also show that there are no periodic states.

6.10.1 Corollary. *All states are cospectral in the bipartite walk defined on the incidence graph of $GQ(s, t)$.*

Proof. We have shown that the transition matrix U lies in the homogeneous coherent algebra $\langle P, Q\rangle$, which implies that U^k has constant diagonal for all k. Since each spectral idempotent E_r of U is a polynomial in U and hence, the matrix E_r^k has constant diagonal for all integer k. □

6.10.2 Lemma. *The average mixing matrix $\widehat{M_U}$ lies in the homogeneous coherent algebra $\langle P, Q\rangle$.*

Proof. Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix. From Equation 6.8.3, we know that U is a linear combination of

$$\{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\}.$$

Each spectral idempotent E_r is a polynomial in U, so we can also write

$$E_r = \sum_{i=1}^{8} \alpha_i^{(r)} M_i,$$

where $\sum M_i = J$ and $M_i \circ M_j = \delta_{i,j} M_i$. So we can write

$$\widehat{M_U} = \sum_r E_r \circ \overline{E_r} = \sum_r \sum_{s=1}^{8} \left|\alpha_i^{(r)}\right|^2 M_i. \qquad \square$$

Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix. Two states e_a and e_b are *strongly cospectral* if for all r,

$$E_r e_a = \mu_r E_r e_b,$$

for some constant μ_r with $|\mu_r| = 1$.

6.10.3 Corollary. *There are no pairs of strongly cospectral states in the bipartite walk defined on the incidence graph of $GQ(s,t)$.*

Proof. Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix. Assume that f_i, f_j are strongly cospectral. Then the average mixing matrix $\widehat{M_U}$ must satisfy that

$$\widehat{M_U} e_i = \widehat{M_U} e_j.$$

By Lemma 6.10.2, two flags f_i, f_j are strongly cospectral if and only if

$$M_k e_i = M_k e_j$$

for all $k \in \{1,2,3,4,5,6,7,8\}$, which implies that a flag f_u is M_k-associated with flag f_i if and only if the flag f_u is also M_k-associated with flag f_j. Now consider M_2, where $(M_2)_{i,j} = 1$ if and only if two distinct flags f_i, f_j share the same block. Since two different flags cannot have the exact same set of "cellmates" in their blocks, for $i \neq j$, there must exist a flag f_u such that

$$(M_2)_{u,i} \neq (M_2)_{u,j}$$

So $M_2 e_i \neq M_2 e_j$ for any $i \neq j$. Thus, we can conclude that there are no strongly cospectral pairs of states in bipartite walks defined over incidence graphs of generalized quadrangles. $\square$

6.10.4 Theorem. *There are no periodic states in the bipartite walk obtained from the incidence graph of a generalized quadrangle.*

Proof. Let $U = \sum_r \theta_r e^{i\theta_r} E_r$ be the spectral decomposition of the transition matrix of the walk. By Corollary 6.10.1, we know the eigenvalue support of a state consists of all the eigenvalues of U. Note that U has only two complex eigenvalues $e^{\pm i\theta}$. By Theorem 5.1.1, we know the walk has a periodic state if and only if

$$\theta \in \mathbb{Q}\pi.$$

In section 6.7, we have shown that $\cos\theta = 2(s+t)-1$, which is an integer. Since $\cos\theta$ is an integer, by Lemma 5.3.2, we can conclude that U has a periodic state if and only if

$$2(s+t)-1 = 0 \text{ or } \pm 1.$$

Since s, t are both positive integers, we know $2(s+t)-1 \neq 0$ or ± 1. □

6.11 Summary

We have looked at both bipartite walks on the incidence graphs of t-designs with $t \geq 2$ and bipartite walks on the incidence graphs of generalized quadrangles $GQ(s,t)$.

Let $\mathcal{D}$ be a t-design $\mathcal{D}$ with parameters (v, b, r, k, λ_t) and G is the incidence graph of $\mathcal{D}$. we define the bipartite walk on G and let U be the transition matrix of the walk.

The incidence matrix N of the design satisfies that

$$NN^T = (r-\lambda_2)I + \lambda_2 J$$

has two eigenvalues $\{rk, r-\lambda_2\}$, which enables us to derive a nice formula for the Hamiltonian of U:

$$H = -\theta \frac{2i}{\sin(\theta)}(PQ - QP) = -\frac{2\theta i}{\sin(\theta) rk} A(\overrightarrow{H}).$$

We define relations between flags of designs, which is a more refined version of the relations introduced by Chakravarti in [7]. Using the relations defined between flags, we know that

(i) The H-digraph is Eulerian with

$$\text{in-degree}(v) = \text{out-degree}(v) = (k-1)(r-\lambda_2)$$

for every vertex v;

(ii) the H-digraph is weakly connected if and only if it is strongly connected;

(iii) if G has girth $2d \geq 6$, then H-graph has diameter two and girth d.

If the design $\mathcal{D}$ is symmetric, then the adjacency matrix of the H-graph is a polynomial in $\{I, A(LG), A(LG_2)\}$ where $A(LG_i)$ is the adjacency matrix of the i-th distance graph of the incidence graph G of $\mathcal{D}$. Moreover, we are able to show that if G has girth ≥ 6, i.e., G is the incidence graph of a projective plane, the H-graph is exactly the distance-2 graph of the line graph of the incidence graph G.

In terms of the behavior of the bipartite walk on a symmetric design, we show that the average mixing matrix $\widehat{M_U}$ satisfies that

$$\widehat{M_U} \in \langle I, A(LG), A(LG_2), A(LG_3) \rangle$$

and we give a bound on the diagonal entries

$$\left(\widehat{M_U}\right)_{i,i} \geq \frac{1}{3},$$

which immediately tells us that there is no uniform average mixing in the bipartite walks on t-designs. We also shows that there are no periodic states in bipartite walks on non-trivial designs.

Another incidence structure we have looked at in this chapter is generalized quadrangles $GQ(s,t)$, which is a 1-(v,k,λ) with $k = s+1, r = t+1$. The incidence matrix N of $GQ(s,t)$ satisfies that NN^T has exactly two non-zero eigenvalues, which allows us to have a formula for the Hamiltonian of U^2:

$$H = -\frac{4\theta i}{\sin(\theta)}(PQ - QP) = -\frac{4\theta i}{\sin(\theta)} \frac{1}{(s+1)(t+1)} A(\overrightarrow{H}).$$

Note that the adjacency matrix of the incidence graph of $GQ(s,t)$ is not invertible. As stated in Section 2.3, we study the Hamiltonian H of U^2 and its corresponding H-graph and H-digraph when the underlying graph is the incidence graph of $GQ(s,t)$.

Let P, Q be the orthogonal projections we get when we define the bipartite walk on $GQ(s,t)$. Then we show that $\langle P, Q \rangle$ is a homogeneous coherent algebra and

$$U, H, A(\overrightarrow{H}), A(H) \in \langle P, Q \rangle.$$

Consequently, there is an unique mutually orthogonal (with respect to Schur multiplication) basis of $\langle P, Q\rangle$ that consists of 01-matrices:

$$\{M_1, M_2, M_3, M_4, M_5, M_6, M_7, M_8\},$$

where each M_i corresponds to a relation between flags described in Section 6.8. Define matrices

$$A_0 = M_1, \quad A_1 = M_2 + M_3, \quad A_2 = M_4 + M_5, \quad A_3 = M_6 + M_7, \quad A_4 = M_8.$$

We show that If $s = t$, then

$$\mathcal{A} = \{A_0, A_1, A_2, A_3, A_4\}$$

forms an association scheme.

In terms of behavior of the bipartite walk on $GQ(s,t)$, using that $U, \widehat{M_U} \in \langle P, Q\rangle$, we show that all states are cospectral but there are no pairs of strongly cospectral states in the walk. There are no periodic states in the walk as well.

6.12 Open questions

Recall that in Theorem 6.5.1, given the transition matrix U of a discrete quantum walk, where $U = \sum_r e^{i\theta_r} E_r$, the average mixing matrix of U is

$$\widehat{M_U} = \sum_r E_r \circ \overline{E_r}.$$

Average mixing matrices in the context of continuous quantum walks also can be defined in a similar way. That is, if the transition matrix U of a continuous quantum walk has spectral decomposition $U(t) = \sum_r e^{i\theta_r t} E_r$, then the average mixing matrix is

$$\widehat{M} = \sum_r E_r^{\circ 2}.$$

Many properties of average mixing matrices of discrete walks also hold for those of continuous walks. Here are some examples:

(i) [20, Lemma 4.5.1] The average mixing matrix is positive semidefinite and all its eigenvalues lie in $[0, 1]$;

(ii) [20, Theorem 4.5.7] If the entries of U are rational, then the entries of $\widehat{M}_U$ are also rational.

Despite all the similarity, there is one property of average maxing matrices of continuous walks that does not hold for those of bipartite walks. In Lemma 2.2 in [17], Godsil proved that in a continuous quantum walk, if the underlying graph is connected, then all the entries of the average mixing matrix are positive. This does not hold for bipartite walks. There are bipartite walks whose average mixing matrices have zero entries while the underlying graphs and their corresponding H-digraph are both connected. For example, bipartite walks on the incidence graph of the projective plane of order n. The incidence graph is connected and the resulting H-digraph is strongly connected. But the average mixing matrix has multiple zero entries on each row.

We ask the following questions:

1. Why is there an entry of zero in $\widehat{M}_U$ when the underlying graph is connected?
2. If $\widehat{M}_{i,j} = 0$, does this give us any combinatorial information? If so, what is the information?

To answer the first question, we note that the average mixing matrix of a bipartite walk is the same as the average mixing matrix of the continuous walk on its H-digraph. To answer the question, we need to study the average mixing matrix for continuous walks on digraphs.

We think Theorem 2.1 in [21] will be helpful in solving the question. Let $\overrightarrow{H}$ be a digraph with skew-adjacency matrix $A(\overrightarrow{H})$. Let $W = u_1 u_2 \cdots u_k$ be a walk joining vertices u_1 and u_k and it is possible that $u_i = u_j$ for $i \neq j$. The sign of the walk W is

$$\prod_{i=1}^{k-1} A(\overrightarrow{H})_{i,i+1}.$$

6.12.1 Theorem (Theorem 2.1 in [21]). *Let $A(\overrightarrow{H})$ be the skew-adjacency matrix of a digraph $\overrightarrow{H}$ and u, v be two arbitrary vertices of D. Let $w^+_{uv}(k)$ denote the number of positive walks between u and v of length k and $w^-_{uv}(k)$ denote the number of negative walks between u and v of length k. Then*

$$A(\overrightarrow{H}^k_{u,v} = w^+_{uv}(k) - w^-_{uv}(k),$$

holds for any non-negative integer k. □

For the second question we posted, our observation on bipartite walks over symmetric designs with $r, k \neq 4$ may help. Let U be the transition matrix of the walk. We observe that

$$\left(\widehat{M_U}\right)_{u,v} = 0$$

if and only if the corresponding flag u and flag v are 3-associated.

Another piece of information we get from the average mixing matrix is about strongly cospectral states. Let $U = \sum_r e^{i\theta_r} E_r$ be the transition matrix. Recall that we say two states e_a and e_b are strongly cospectral if for all r,

$$E_r e_a = \mu_r E_r e_b,$$

for some constant μ_r with $|\mu_r| = 1$. Being strongly cospectral is a necessary condition for two states to have perfect state transfer. The study of strongly cospectral states has attracted a lot of attention [4, 13, 33].

Using average mixing matrices, Godsil provided another definition of strongly cospectral states.

6.12.2 Theorem (Theorem 9.3 in [17])**.** *In continuous quantum walks, two states e_a and e_b are strongly cospectral if and only if $\widehat{M_U} e_a = \widehat{M_U} e_b$.* □

The statement in the theorem above also holds when the walk is a bipartite walk. The proof of the theorem can be easily adapted to the case of bipartite walks, so we omit the proof here.

But there is not much study about strongly cospectral states that are done using the approach of average mixing matrices. We think using average mixing matrices is a promising approach and it may help to reveal combinatorial relation between strongly cospectral pairs.

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