# Discrete Quantum Walks on Graphs and Digraphs

by

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

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# Abstract

This thesis studies various models of discrete quantum walks on graphs and digraphs via a spectral approach.

A discrete quantum walk on a digraph $X$ is determined by a unitary matrix $U$, which acts on complex functions of the arcs of $X$. Generally speaking, $U$ is a product of two sparse unitary matrices, based on two direct-sum decompositions of the state space. Our goal is to relate properties of the walk to properties of $X$, given some of these decompositions.

We start by exploring two models that involve coin operators, one due to Kendon, and the other due to Aharonov, Ambainis, Kempe, and Vazirani. While $U$ is not defined as a function in the adjacency matrix of the graph $X$, we find exact spectral correspondence between $U$ and $X$. This leads to characterization of rare phenomena, such as perfect state transfer and uniform average vertex mixing, in terms of the eigenvalues and eigenvectors of $X$. We also construct infinite families of graphs and digraphs that admit the aforementioned phenomena.

The second part of this thesis analyzes abstract quantum walks, with no extra assumption on $U$. We show that knowing the spectral decomposition of $U$ leads to better understanding of the time-averaged limit of the probability distribution. In particular, we derive three upper bounds on the mixing time, and characterize different forms of uniform limiting distribution, using the spectral information of $U$.

Finally, we construct a new model of discrete quantum walks from orientable embeddings of graphs. We show that the behavior of this walk largely depends on the vertex-face incidence structure. Circular embeddings of regular graphs for which $U$ has few eigenvalues are characterized. For instance, if $U$ has exactly three eigenvalues, then the vertex-face incidence structure is a symmetric 2-design, and $U$ is the exponential of a scalar multiple of the skew-symmetric adjacency matrix of an oriented graph. We prove that, for

every regular embedding of a complete graph, $U$ is the transition matrix of a continuous quantum walk on an oriented graph.

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# Contents

# Chapter 1

# Introduction

Quantum walks have become important tools for designing quantum algorithms. Grover's search [38] can be viewed a quantum walk on the complete graph with loops. Ambainis's algorithm for element distinctness [3] is equivalent to a quantum walk on the Johnson graph. For many problems, quantum walk based algorithms outperform their classical counterparts.

There are two classes of quantum walks—continuous quantum walks and discrete quantum walks, depending on how the system evolves.

A continuous quantum walk has a simple definition: for a graph $X$, the quantum states are complex functions on its vertices, and the transition matrix is

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

where $H$ is the adjacency matrix or the Laplacian matrix of $X$. Thus, the behavior of a continuous quantum walk can be analyzed using the spectral information of the graph.

For a discrete quantum walk, however, there is no simple definition that takes place on the vertex set of the graph. The current trend is to enlarge the state space to complex functions on the arcs. We illustrate one example, constructed by Aharonov, Ambainis, Kemp, and Vazirani [2], on a cycle. Our walker is endowed with two states: the position state, which indicates the vertex she stands on, and the coin state, which tells her the direction to move in. A step of the walk consists of a coin flip followed by a shift operation. The coin flip maps her current direction to a superposition of both clockwise and counterclockwise directions, and the shift operator moves her one step towards the directions given by the coin state. In other words, $U$ is a product of two sparse unitary matrices $U_1$ and $U_2$, both indexed by the arcs of the cycle. There are variants of this walk; for example, the shift operator can be replaced by an arc-reversal operator, as proposed by Kendon [46]. A model that generalizes the example in Aharonov et al [2] will be called a shunt-decomposition model, and a model that generalizes Kendon's example will be called an arc-reversal model.

The purpose of this thesis is to study discrete quantum walks on general graphs. While the definition of a discrete quantum walk is intuitive, exact analysis could be very difficult to carry out. The shunt-decomposition walk on the infinite path, studied by Ambainis, Bach, Nayak, and Vishwanath [4], exhibits striking differences compared to the classical random walk, but these properties are proved via complicated recurrences. For graphs with higher valency, this method might not be as effective. Following techniques used in continuous quantum walks, one can instead investigate a discrete quantum walk from the spectral decomposition of $U$. However, this is also not easy. On one hand, since $U_1$ and $U_2$ do not commute, their spectra have no direct impact on the spectrum of $U$. On the other hand, the extra coin space makes the connection between $U$ and $X$ even more obscure. Is it even possible to analyze discrete quantum walks using graph spectra?

Our first contribution clears the above doubt. Although $U$ is not defined in terms of the adjacency matrix $A$, many properties of the above walks turn out to solely depend on $A$. This leads to a characterization of rare phenomena, such as perfect state transfer and uniform average vertex mixing, in the language of algebraic graph theory. For instance, in an arc-reversal walk on a regular graph, perfect state transfer occurs from vertex $u$ to $v$ if and only if $u$ and $v$ are strongly cospectral, and their eigenvalue support satisfies some algebraic conditions (Theorem 2.5.3). As another example, in a shunt-decomposition walk on a certain Cayley digraph $X$, the eigenvalues of $U$ are roots of polynomials whose coefficients are eigenvalues of $X$ (Theorem 4.3.7). We show that for every prime $p$, a 3-regular circulant digraph over $\mathbb{Z}_p$ admits uniform average vertex mixing if and only if its automorphism group coincides with $\mathbb{Z}_p$ (Theorem 4.4.4). Our characterization yields infinitely many examples with valency greater than two, while previous examples were mostly variants of cycles. This part is done in Chapter 2 and Chapter 4; it extends the work on two current models.

The second theme of our thesis is the study of more abstract quantum walks. Due to the choice of shift operator and coins, on the same graph, many different discrete quantum walks can be defined. Yet, this does not stop people from constructing new models, say Szegedy's quantization of

Markov chains [59], and the staggered walks due to Portugal, Santos, Fernandes, and Goncalves [56]. A unifying language that describes common properties of all quantum walks is thus needed. In Chapter 3, we investigate an abstract quantum walk, with no extra assumption on $U$. We show that knowing the spectral decomposition of $U$ leads to a better understanding of the limiting distribution. In particular, we obtain three new bounds on the mixing time (Theorem 3.3.1), all tighter than the bound in [2]. We also study when the limiting distribution is uniform over the arcs and over the vertices. We prove that the latter is implied by the former (Theorem 3.4.5), while the former happens if and only if $U$ has simple eigenvalues and flat eigenprojections (Theorem 3.4.4). Finally, some algebraic properties of the average mixing matrix are derived (Theorem 3.4.6 and Theorem 3.4.7), motived by their successful application in continuous quantum walks. The results in this chapter are applied to specific models later.

In the last part of the thesis, we construct and study a new model, called vertex-face walks, based on orientable embeddings. It is a variant of the arc-reversal walk on $X$—at every other step, the walk takes place on the dual graph $X^*$, that is, the graph with faces of $X$ as vertices, and two vertices are adjacent in $X^*$ if the corresponding faces share an edge in $X$. The vertices of $X^*$ are the faces of $X$, and two vertices of $X^*$ are adjacent if they correspond to faces of $X$ that share an edge. This model may seem to violate the locality condition, proposed by Aaronson and Ambainis [1], when viewed as a discrete quantum walk on $X$. However, there are search algorithms that effectively use the vertex-face walk for a toroidal embedding of $C_n \square C_n$ [6, 23, 55]. On the other hand, we may interpret $U$ as a quantum walk that satisfies the locality criterion on a different digraph. Consider the following process: given a graph $X$, construct an orientable embedding $\mathcal{M}$; given the embedding $\mathcal{M}$, build the transition matrix $U$ of a vertex-face walk; given the matrix $U$, compute a Hermitian matrix $H$ such that $U = \exp(iH)$; and given $H$, find the underlying digraph $Z$. A question arises: for which embedding $\mathcal{M}$ is the digraph $Z$ sparse, with very few weights on the arcs assigned by $H$? If a discrete quantum walk satisfies this condition, then we can implement it as a continuous quantum walk on a digraph. Using the spectral decomposition of $U$, we find interesting relations between the walk and the embedding, which provide answers to the above question. For example, if the vertex-face incidence structure is a symmetric 2-design, then $U$ is the transition matrix of a continuous quantum walk on an oriented graph (Theorem 5.4.3). We then obtain infinitely many examples from regular embeddings of complete graphs (Theorem 5.6.3).

Below we give a more detailed description of the main results in each part.

## 1.1 Extending Work in Current Models

Let $X$ be a $d$-regular graph on $n$ vertices. We replace each edge $\{u, v\}$ with two arcs $(u, v)$ and $(v, u)$. A quantum state associated with $X$ is a complex function on its arcs. These states form a vector space, isomorphic to $\mathbb{C}^n \otimes \mathbb{C}^d$. Parallel vectors in $\mathbb{C}^n \otimes \mathbb{C}^d$ are identified as the same state; we will pick one with unit length as the representative.

A discrete quantum walk is determined by a unitary matrix $U$ acting on $\mathbb{C}^n \otimes \mathbb{C}^d$. At step $k$, the system is in state

$$x_k := U^k x_0,$$

given initial state $x_0$. We call $U$ the transition matrix of the quantum walk.

In this section, we highlight our contributions to the areas of two quantum walks, proposed by Kendon [46] and Ahaoronov et al [2]. These models will be referred to as the arc-reversal model and the shunt-decomposition model, respectively. In both cases, the transition matrix is a product of two matrices—one acts on a subspace isomorphic to $\mathbb{C}^d$, and the other permutes the arcs of $X$.

Let $R$ be the permutation matrix that sends arc $(u, v)$ to arc $(v, u)$. For each vertex $u$, pick a linear order $f_u$ on the neighbors of $u$. Let $C$ be a $d \times d$ unitary matrix, called the coin. Let $I$ be the identity matrix. An arc-reversal $C$-walk on $X$ is determined by the transition matrix

$$U := R(I \otimes C),$$

whose rows and columns are indexed by the arcs of $X$ in the order

$$f_1(1), \cdots, f_1(d), f_2(1), \cdots, f_2(d), \cdots, f_n(1), \cdots, f_n(d).$$

This model has been widely applied to quantum algorithms, especially in spatial search. A popular choice for $C$ in these algorithms is the Grover coin, named after Grover's search:

$$G = \frac{2}{d} J - I,$$

where $J$ is the all-ones matrix. Note that $G$ commutes with every permutation, so the transition matrix can be written as

$$U = R(I \otimes G),$$

regardless of the linear orders $\{f_u : u \in V(X)\}$. Another observation on the arc-reversal Grover walk is that both $R$ and $I \otimes G$ are involutions, so they represent reflections about two subspaces. A quantum walk whose transition matrix is a product of two reflections was first studied by Watrous [62]. In Section 2.3, we extend his work, and develop theory towards the spectral decomposition of any matrix lying in the algebra generated by two reflections. Using our characterization, we find the spectral relation between $U$ and $X$. The following is a summary of our results in Section 2.4.

**1.1.1 Theorem.** *Let $X$ be a $d$-regular graph on $n$ vertices. Let $U = R(I \otimes G)$ be the transition matrix of the arc-reversal Grover walk on $X$. Let $M$, $D_t$, $D_h$, and $B$ be the arc-edge incidence matrix, tail-arc incidence matrix, head-arc incidence matrix, and vertex-edge incidence matrix of $X$, respectively.*

*(i) The 1-eigenspace of $U$ is*

$$(\operatorname{col}(M) \cap \operatorname{col}(D_t^T)) \oplus (\ker(M^T) \cap \ker(D_t))$$

*with dimension*

$$\frac{nd}{2} - n + 2.$$

*(ii) If $X$ is bipartite, the $(-1)$-eigenspace of $U$ is*

$$M \ker(B) \oplus D_t^T \ker(B^T)$$

*with dimension*

$$\frac{nd}{2} - n + 2.$$

*If $X$ is not bipartite, the $(-1)$-eigenspace of $U$ is*

$$M \ker(B),$$

*with dimension*

$$\frac{nd}{2} - n.$$

*(iii) The multiplicities of the non-real eigenvalues of $U$ sum to $2n - 4$ if $X$ is bipartite, and $2n - 2$ otherwise. Let $y$ be an eigenvector for $X$ with eigenvalue $\lambda \in (-d, d)$. Let $\theta \in \mathbb{R}$ be such that $\lambda = d\cos(\theta)$. Let $\theta \in \mathbb{R}$ be such that $\lambda = d\cos(\theta)$. Then*

$$D_t^T y - e^{i\theta} D_h^T y$$

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

$$D_t^T y - e^{-i\theta} D_h^T y$$

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

The above relation allows us to study properties of quantum walks using properties of the underlying graph. Among all interesting phenomena in quantum walks, perfect state transfer is one that can be analyzed purely in terms of the graph spectra, as we prove in Section 2.5.

Suppose the system starts with a state that "concentrates on" $u$, that is, a complex function that sends all arcs to 0 except for those leaving $u$. Is there a vertex $v$ such that the system concentrates on vertex $v$ at some time $k$? A quantum walk with this phenomenon is said to admit perfect state transfer from $u$ to $v$ at time $k$. The physical interpretation of perfect state transfer is that, after $k$ steps, the walker will be found at vertex $v$ with certainty, given that she started at vertex $u$. Let $e_u$ be the characteristic vector of the vertex $U$. We will consider perfect state transfer from $u$ to $v$ with initial state

$$\frac{1}{\sqrt{d}} e_u \otimes \mathbf{1},$$

which is a column of the coin matrix $I \otimes G$.

Unlike perfect state transfer in continuous quantum walks, discrete perfect state transfer may lose many nice properties such as symmetry, thus the theory developed for continuous quantum walk (see for example [27]) does not necessarily carry over. Surprisingly, in the arc-reversal walk, some of these properties stay, and we can determine perfect state transfer by looking at $X$ only.

**1.1.2 Theorem** (2.5.3). *Let $X$ be a $d$-regular graph, with spectral decomposition*

$$A = \sum_{\lambda} \lambda E_{\lambda}.$$

*Then the arc-reversal Grover walk on $X$ admits perfect state transfer from $u$ to $v$ at time $k$ if and only if all of the following hold.*

*(i) For each $\lambda$, we have $E_\lambda e_u = \pm E_\lambda e_v$.*

*(ii) If $E_\lambda e_u = E_\lambda e_v \neq 0$, then there is an even integer $j$ such that*

$$\lambda = d\cos(j\pi/k).$$

*(iii) If $E_\lambda e_u = -E_\lambda e_v \neq 0$, then there is an odd integer $j$ such that*

$$\lambda = d\cos(j\pi/k).$$

□

A pair of vertices $(u, v)$ satisfying condition (i) is said to be strongly cospectral. In continuous quantum walks, strong cospectrality is also a necessary condition for perfect state transfer, and has been thoroughly studied since Coutinho's Ph.D. thesis [17]. Conditions (ii) and (iii), however, are more restrictive compared to the eigenvalue conditions for continuous perfect state transfer, since the time steps here are integers. Using tools from algebraic graph theory, we construct an infinite family of examples with perfect state transfer in arc-reversal walks. This is the first infinite family of graphs, other than cycles, that admit perfect state transfer.

**1.1.3 Theorem** (2.5.7)**.** *Let $\ell$ be an odd integer. For any distinct integers $a$ and $b$ such that $a+b=\ell$, the arc-reversal Grover walk on the circulant graph $X(\mathbb{Z}_{2\ell}, \{a, b, -a, -b\})$ admits perfect state transfer at time $2\ell$ from vertex $0$ to vertex $\ell$.* □

We now move on to the second type of quantum walks. In a shunt-decomposition walk, the walker preserves her direction when moving between adjacent vertices. On infinite paths or grids, these directions are naturally defined. To generalize the definition, we show that specifying directions on a digraph is equivalent to decomposing its adjacency matrix into permutation matrices, called shunts:

$$A = P_1 + \cdots + P_d.$$

Here, each shunt $P_j$ maps a vertex to one of its neighbors, and represents a direction on the graph $X$. If $S$ is the permutation matrix given by

$$S = \begin{pmatrix} P_1^{-1} & & & \\ & P_2^{-1} & & \\ & & \ddots & \\ & & & P_d^{-1} \end{pmatrix},$$

then the transition matrix of a shunt-decomposition walk is

$$U := S(C \otimes I).$$

Note here $U$ acts on $\mathbb{C}^d \otimes \mathbb{C}^n$, and the linear orders $\{f_u : u \in V(X)\}$ are determined implicitly by the ordered shunts $(P_1, P_2, \ldots, P_d)$.

The main purpose of Chapter 4 is to study interesting phenomena that happen on shunt-decomposition walks. For $S$ with order greater than two, we lack the machinery to deal with the algebra $\langle S, C \otimes I\rangle$. Thus, most of Chapter 4 is devoted to special walks where all shunts commute. In this case, $X$ is a Cayley graph over some abelian group $\Gamma$.

It is shown by Aharonov et al [2] that, for Cayley graphs over abelian groups, the eigenvalues and eigenvectors of $U$ are determined by the coin $C$ together with the characters of $\Gamma$. However, computing the eigenvalues of $U$ still remains a non-trivial task. We apply their result to walks with the Grover coin $G$, and find explicit formulas for the eigenvalues and eigenvectors of $U$.

**1.1.4 Theorem.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. For each character $\chi$ of $\Gamma$, let*

$$\Lambda_\chi = \begin{pmatrix} \chi(g_1^{-1}) & & & \\ & \chi(g_2^{-1}) & & \\ & & \ddots & \\ & & & \chi(g_d^{-1}) \end{pmatrix}.$$

*The eigenvalues of $U$ consists of eigenvalues of $\Lambda_\chi G$, where $\chi$ ranges over all characters of $\Gamma$. Moreover, each eigenvalue $\alpha$ of $\Lambda_\chi G$ is either*

*(i) a zero of*

$$\frac{1}{\alpha\chi(g_1)+1} + \cdots + \frac{1}{\alpha\chi(g_d)+1} - \frac{d}{2},$$

*with multiplicity 1, or,*

*(ii) $-\chi(g_j^{-1})$, with multiplicity one less than the number of $k$'s such that $\chi(g_k) = \chi(g_j)$.* □

We study a question concerning the limiting distribution: is there a quantum walk, such that whatever state the walker starts with, in the time-averaged limit, she will be found on any vertex with equal probability? This phenomenon is called uniform average vertex mixing. Aharonov et al [2] showed that uniform average vertex mixing happens if $U$ has simple eigenvalues. Using this criterion, they proved that every odd cycle with the Hadamard coin admits uniform average vertex mixing.

We seek examples with higher valency. With the Grover coin, however, $U$ will never have distinct eigenvalues, so the above criterion does not apply. Fortunately, uniform average vertex mixing can still happen with a slightly weaker condition, as we show in the following theorem.

**1.1.5 Theorem** (4.3.3)**.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. If the only non-simple eigenvalue of $U$ is $-1$ with multiplicity $d-1$, then $U$ admits uniform average vertex mixing.* □

This opens up possibilities for more examples. Given our formulas for the eigenvalues of $U$, we find a close connection between uniform average vertex mixing and the algebraic properties of the digraph. Contrary to our intuition, uniform average vertex mixing is more likely to happen on a Cayley digraph with as few symmetries as possible. In particular, we show that for every prime $p$, a 3-regular circulant digraph over $\mathbb{Z}_p$ admits uniform average vertex mixing if and only if its automorphism group is the smallest possible, that is, $\mathbb{Z}_p$.

**1.1.6 Theorem** (4.4.4)**.** *Let $p$ be a prime. Let $X$ be a 3-regular circulant digraph over $\mathbb{Z}_p$. Then the shunt-decomposition Grover walk on $X$ admits uniform average vertex mixing if and only if its connection set has trivial stabilizer in* $\mathrm{Aut}(\mathbb{Z}_p)$. □

## 1.2 Analyzing Abstract Quantum Walks

For this part, we assume $X$ is a digraph, and $U$ is simply a unitary matrix indexed by the arcs of $X$. In Chapter 3, we analyze the abstract walk on $X$, and characterize the limiting behavior using the spectral decomposition of $U$, say

$$U = \sum_r e^{i\theta_r} F_r.$$

The language we use in this chapter differs a bit from the literature, in two ways.

(i) Most results are stated in terms of a subset of the arcs. This avoids distinguishing between the probability that the walker is on an arc and the probability that she is on a vertex.

(ii) The evolution is phrased in the density matrix formalism. This yields cleaner formulas for many parameters we are interested in.

A density matrix is a positive semidefinite matrix $\rho$ with $\operatorname{tr}(\rho) = 1$. It represents a pure state if $\rho = xx^*$ for some unit vector $x$, and represents a mixed state otherwise. For example,

$$\rho = e_a e_a^T$$

is the density matrix for a pure state concentrated on the arc $a$, and

$$\rho_S := \frac{1}{|S|} \sum_{a \in S} e_a e_a^T$$

represents the uniform mixed state over the arcs in $S$.

Suppose the system is initialized to some state $\rho_0$. Then, at step $k$, it is in state

$$\rho_k := U^k \rho_0 (U^k)^*.$$

Let $\langle \cdot, \cdot \rangle$ be the usual inner product of complex vectors. If we perform a measurement in the standard basis, then the system collapses to state $e_a e_a^T$ with probability

$$P_{\rho_0,a}(k) = \langle \rho_k, e_a e_a^T \rangle.$$

In general, the probability that the walker is on $S$ at time $k$ is

$$P_{\rho_0,S}(k) = |S| \langle \rho_k, \rho_S \rangle.$$

We investigate the limiting behavior of the state $\rho_k$ and the probability $P_{\rho_0,S}(k)$. Since the evolution is unitary, these two quantities do not converge as $k$ tends to infinity. However, their Cesàro sums exist, and can be expressed using the spectral decomposition of $U$. We will call these two limits the average state and the average probability.

**1.2.1 Theorem** (3.2.2)**.** *Let $U$ be a unitary matrix with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*Given initial state $\rho_0$, the average state of the quantum walk with $U$ as the transition matrix is*

$$\lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} \rho_k = \sum_r F_r \rho_0 F_r. \qquad 53$$

**1.2.2 Theorem** (3.2.3)**.** *Let $X$ be a digraph. Let $U$ be a transition matrix of a quantum walk on $X$, with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*Given initial state $\rho_0$ and a subset $S$ of arcs, the average probability of the quantum walker being on $S$ is*

$$\lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k) = |S| \sum_r \langle F_r \rho_0 F_r, \rho_S\rangle. \qquad \square$$

We then study two questions about the limit $|S|\sum_r \langle F_r \rho_0 F_r, \rho_S\rangle$: how fast is it approached, and when does it depend only on the size of $S$? Both properties play a role in quantum walk based algorithms.

The first property is quantified by the mixing time $M_{\rho_0,S}(\epsilon)$, that is, the smallest time step $L$ such that for all $K > L$,

$$\frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k)$$

is $\epsilon$-close to the limit. We prove four upper bounds on the mixing time; the last one was first found by Aharonov et al [2]. Clearly, the more spectral information we have about $U$, the tighter bound we obtain.

**1.2.3 Theorem** (3.3.1)**.** *Let $X$ be a digraph. Let $U$ be a transition matrix of a quantum walk on $X$, with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*Given initial state $\rho_0$ and a subset $S$ of arcs, the mixing time $M_{\rho_0,S}(\epsilon)$ satisfies*

$$\begin{aligned} M_{\rho_0,S}(\epsilon) &\le \frac{2|S|}{\epsilon} \sum_{r \ne s} \frac{|\langle F_r \rho_0 F_s, \rho_S \rangle|}{|e^{i\theta_r} - e^{i\theta_s}|} \\ &\le \frac{2}{\epsilon} \sum_{r \ne s} \sum_{a \in S} \frac{\sqrt{(F_r)_{aa}(F_s)_{aa}}}{|e^{i\theta_r} - e^{i\theta_s}|} \\ &\le \frac{2|S|}{\epsilon} \sum_{r \ne s} \frac{1}{|e^{i\theta_r} - e^{i\theta_s}|} \\ &\le \frac{2\ell |S|}{\epsilon \Delta}, \end{aligned}$$

*where $\ell$ is the number of pairs of distinct eigenvalues, and*

$$\Delta := \min\{ \left| e^{i\theta_r} - e^{i\theta_s} \right| : r \ne s \}. \qquad \square$$

The second question asks for a uniform limiting distribution. Suppose $X$ has $n$ vertices and $m$ arcs. We say $U$ admits uniform average mixing if

$$|S| \sum_r \langle F_r \rho_0 F_r, \rho_S \rangle = \frac{1}{m}$$

for every subset $S$ of size one, and $U$ admits uniform average vertex mixing if

$$|S| \sum_r \langle F_r \rho_0 F_r, \rho_S \rangle = \frac{1}{n}$$

for every subset $S$ that consists of all the outgoing arcs of some vertex. The following results in Theorem 3.4.4 characterize uniform average mixing. We say a matrix is *flat* if all its entries have the same absolute value.

**1.2.4 Theorem.** *Let $U$ be a transition matrix on a digraph $X$. Uniform average mixing occurs if and only if $U$ has simple eigenvalues with flat eigenprojections.* $\square$

Uniform average mixing also implies something stronger, including uniform average vertex mixing.

**1.2.5 Theorem** (3.4.5)**.** *Let $X$ be a digraph. If a quantum walk on $X$ admits uniform average mixing, then for any initial state $\rho_0$ and any arc set $S$,*

$$\lim_{K \to \infty} \frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k) = \frac{|S|}{nd}. \qquad \square$$

We also prove some algebraic properties of the mixing matrix

$$\widehat{M} = \lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} U^k \circ \overline{U^k},$$

which records the average probabilities from arcs to arcs. The following results appear in Theorem 3.4.6 and Theorem 3.4.7.

**1.2.6 Theorem.** *If the entries of $U$ are algebraic over $\mathbb{Q}$, then the entries of $\widehat{M}$ are algebraic over $\mathbb{Q}$. If the entries of $U$ are rational, then the entries of $\widehat{M}$ are rational.*

## 1.3 Exploring Walks from Embeddings

The idea of alternating operators in a quantum walk is not new. Patel, Raghunathan and Rungta [55] and Falk [23] both proposed quantum walk based search algorithms, where different operators are applied at even and odd steps. Ambainis, Portugal and Nahimov [6] then studied this type of algorithm analytically, showing its performance matches other type of quantum walks.

The algorithm in [6] searches a marked vertex on a 2-dimensional grid, which can be viewed as a Cartesian square of a cycle:

$$X := C_n \square C_n.$$

If we remove the oracle from the algorithm, then the two operators are reflections based on two partitions of the vertices, illustrated by the blue squares and red squares in Figure 1.1. The transition matrix is indexed by $V(X)$.

We notice that Figure 1.1 represents a graph self-dual embedding of $C_n \square C_n$ on the torus. In fact, it gives rise to an embedding of another graph $Y$, obtained by truncating the edges of $X$ and joining the new vertices by blue and red edges, as shown in Figure 1.2.

Note that $Y$ is isomorphic to $C_{2n} \square C_{2n}$, and the blue and red squares partition $V(Y)$ in the same way as in Figure 1.1. Thus according to [6], there is a transition matrix $U$, indexed by $V(Y)$, which arises from these partitions. On the other hand, we may think of the vertices of $Y$ as arcs of $X$—the one closer to $u$ on edge $\{u, v\}$ is the arc $(u, v)$, with tail $u$. Now, the blue squares partition the arcs based on their tails, while the red squares

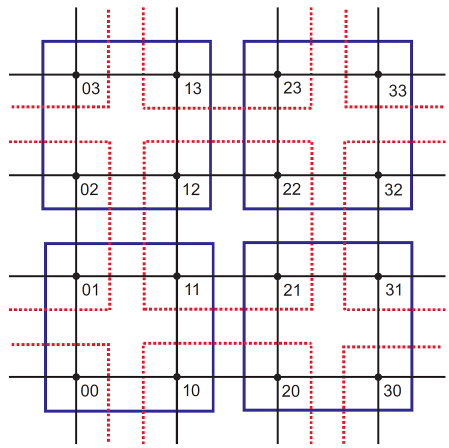



Figure 1.1: Two partitions of the vertices of $C_n \square C_n$

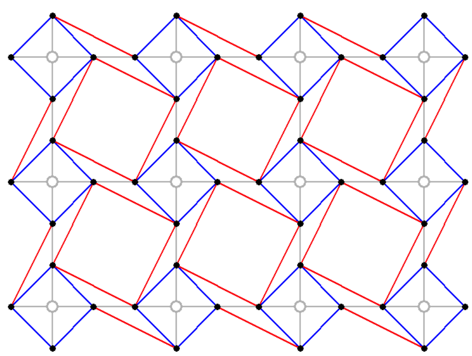


Figure 1.2: Two partitions of the arcs of $C_n \square C_n$

partition the arcs based on the faces they lie in. In this sense, $U$ is a transition matrix of $X$, indexed by its arcs.

We generalize the above idea to any orientable embedding. Let $X$ be a graph, and $\mathcal{M}$ an embedding of $X$ on some orientable surface. Consider a consistent orientation of the faces, that is, whenever an edge is shared by two faces $f$ and $h$, the direction it receives in $f$ is opposite to the direction it receives in $h$. In such an orientation, every arc belongs to exactly one face; let $M$ be the associated arc-face incidence matrix. We also group arcs based on their tails, and let $N$ be the associated arc-tail incidence matrix. To construct a unitary matrix, let $\widehat{M}$ and $\widehat{N}$ be the matrices obtained from

$M$ and $N$ by scaling each column to a unit vector, and set

$$U := (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I).$$

Here $\widehat{M}\widehat{M}^T$ is the orthogonal projection onto the column space $\operatorname{col}(\widehat{M})$, and $2\widehat{M}\widehat{M}^T - I$ is the reflection about $\operatorname{col}(\widehat{M})$. A quantum walk with $U$ as the transition matrix is called the vertex-face walk, relative to some consistent orientation of $\mathcal{M}$.

We study vertex-face walks in Chapter 5, mainly focused on the relation between properties of the walk and properties of the embedding.

The first thing we notice is that, a vertex-face walk for $\mathcal{M}$ can be viewed as two arc-reversal walks, one on the original graph $X$, and one on the dual graph $X^*$. In fact, we have observed that for some graph self-dual embeddings, the transition matrix of the vertex-face walk is permutation similar to the square of the transition matrix of the arc-reversal walk.

The second contribution is the spectral decomposition of $U$; this is done using techniques in Section 2.3, since $U$ is a product of two reflections. It turns out that the spectrum of $U$ is determined by the spectrum of the vertex-face incidence matrix, which contains important information of the embedding. We summarize below the results on circular embeddings, that is, embeddings where every face is bounded by a cycle.

**1.3.1 Theorem.** *Let $\mathcal{M}$ be a circular embedding of a connected graph with $n$ vertices, $\ell$ edges and $s$ faces on an orientable surface of genus $g$. Let $U$ be a transition matrix of the vertex-face walk for $\mathcal{M}$. Let $\widehat{M}$ and $\widehat{N}$ be the normalized arc-face incidence matrix and the normalized arc-tail incidence matrix, respectively. Let $\widehat{C}$ be the normalized vertex-face incidence matrix.*

*(i) The 1-eigenspace of $U$ is*

$$(\operatorname{col}(\widehat{M}) \cap \operatorname{col}(\widehat{N})) \oplus (\ker(\widehat{M}^T) \cap \ker(\widehat{N}^T))$$

*with dimension $\ell + 2g$.*

*(ii) The $(-1)$-eigenspace for $U$ is*

$$\widehat{M}\ker(\widehat{C}) \oplus \widehat{N}^T \ker(\widehat{C}^T)$$

*with dimension*

$$n + s - 2\operatorname{rk}(\widehat{C}).$$

(iii) *The multiplicities of the non-real eigenvalues of* $U$ *sum to* $2\operatorname{rk}(\widehat{C}) - 2$. *Let* $\mu \in (0,1)$ *be an eigenvalue of* $\widehat{C}\widehat{C}^T$. *Choose* $\theta$ *with* $\cos(\theta) = 2\mu - 1$. *The map*
$$y \mapsto (\cos(\theta) + 1)\widehat{N}y - (e^{i\theta} + 1)\widehat{M}\widehat{C}^T y$$
*is an isomorphism from the* $\mu$*-eigenspace of* $\widehat{C}\widehat{C}^T$ *to the* $e^{i\theta}$*-eigenspace of* $U$*, and the map*
$$y \mapsto (\cos(\theta) + 1)\widehat{N}y - (e^{-i\theta} + 1)\widehat{M}\widehat{C}^T y$$
*is an isomorphism from the* $\mu$*-eigenspace of* $\widehat{C}\widehat{C}^T$ *to the* $e^{-i\theta}$*-eigenspace of* $U$. □

Based on the spectral decomposition, we characterize when $U$ has exactly two eigenvalues and three eigenvalues, in Section 5.4.

**1.3.2 Theorem.** *Let* $\mathcal{M}$ *be a circular orientable embedding. Let* $U$ *be the transition matrix of a vertex-face walk for* $\mathcal{M}$.

(i) $U$ *has exactly two eigenvalues if and only if every face is bounded by a Hamilton cycle.*

(ii) *For a circular embedding of a regular graph,* $U$ *has exactly three eigenvalues if and only if the vertex-face incidence structure is a symmetric 2-design.* □

The third part explores possibilities of implementing vertex-face walks as continuous quantum walks. We look for transition matrices $U$ such that $U = \exp(iH)$, where $H$ is sparse and has as few different entries as possible. The following theorems, from Section 5.6 and Section 5.8, provide infinitely many examples.

**1.3.3 Theorem** (5.6.3)**.** *Let* $n$ *be a prime power. Let* $U$ *be the transition matrix of the vertex-face walk for a regular embedding of* $K_n$. *Then there is* $\gamma \in \mathbb{R}$ *such that*
$$U = \exp(\gamma(U^T - U)).$$
*Moreover,* $U^T - U$ *is a scalar multiple of the skew-symmetric adjacency matrix of an oriented graph, which*

(i) *has* $n(n-1)$ *vertices,*

*(ii)* *is* $(n-2)$*-regular, and*

*(iii)* *has exactly three eigenvalues:* $0$ *and* $\pm i\sqrt{n^2-2n}$. □

**1.3.4 Theorem** (5.8.5)**.** *Let* $n$ *be a power of* $2$*. Let* $\mathcal{M}$ *be a regular embedding of* $K_n$*. Let* $\phi$ *be the* $2$*-fold arc-function that sends every arc of* $X$ *to the element* $(1,2) \in \mathrm{Sym}(2)$*. Let* $\mathcal{M}'$ *be the embedding of* $K_2 \times K_n$ *induced by* $(M', \phi)$*. Let* $U'$ *be the transition matrix of the vertex-face walk for* $\mathcal{M}'$*. Then there is* $\gamma \in \mathbb{R}$ *such that*

$$(U')^2 = \exp(\gamma((U')^T - U')).$$

*Moreover,* $(U')^T - U'$ *is a scalar multiple of the skew-symmetric adjacency matrix of an oriented graph, which*

*(i)* *has* $2n(n-1)$ *vertices,*

*(ii)* *is* $(n-2)$*-regular, and*

*(iii)* *has exactly three eigenvalues:* $0$ *and* $\pm 2i\sqrt{n^2-2n}$. □

Finally, in Section 5.9, we show that the above infinite families of vertex-face walks tend to “stay at home”, that is, the probability that the quantum walker stays at the initial state tends to 1 as the size of the graph goes to infinity.

# Chapter 2

# The Simplest Model

A quantum walker moves unitarily on the graph. Her state, as a complex function on the arcs, gets updated by a unitary matrix at each step. Standing on the arc $(u, v)$, our walker decides to move in the simplest way: first, split herself over all outgoing arcs of $u$, with complex weights determined by a coin, and then, move all copies of her to the reversed arcs of where they are. These constitute one iteration of the walk. After several steps, she might be everywhere on the graph, or concentrated on a special subset of arcs.

In this chapter, we give a formal description of the above walk, called the arc-reversal walk, and study its behavior via spectral analysis. The transition matrix of our walk is a product of two non-commuting reflections, that is,

$$U = U_1 U_2,$$

for some Hermitian $U_1$ and $U_2$ with $U_1^2 = U^2 = I$. For any unitary matrix of this type, a complete characterization of its eigenvalues and eigenspaces is given in Section 2.3. These results will be applied again to a different model in Chapter 5.

While the transition matrix $U$ of the arc-reversal walk is not an obvious function in the adjacency matrix of the graph $X$, our analysis in Section 2.4 reveals a strong connection between the graph spectrum and the walk spectrum. In particular, eigenvalues of $X$ provide the real parts of eigenvalues of $U$, and eigenvectors of $X$ can be lifted to eigenvectors of $U$ by two incidence matrices.

This observation enables us to characterize perfect state transfer purely in terms of graph spectra. In Section 2.5, we show that perfect state transfer occurs between two vertices if and only if they are strongly cospectral and the graph eigenvalues satisfy a simple condition. Based on this characterization, we construct an infinite family of 4-regular circulant graphs that admit perfect state transfer. To the best of our knowledge, this is the first infinite family of graphs, other than cycles, that are proved to admit perfect state transfer in discrete quantum walks.

## 2.1 Searching as a Quantum Walk

Suppose that in an unstructured database with $n$ datapoints, exactly one point satisfies some desired property. To locate this point, a naive approach is to select a candidate uniformly at random, and check if it satisfies our criterion. On average, this finds the target in $O(n)$ steps. It turns out that no classical algorithm can do better than this. However, with quantum algorithms, we can pinpoint the target in $O(\sqrt{n})$ steps, as demonstrated by Grover [39].

To understand the quantum approach, we rephrase the above problem as follows. Consider a complex inner product space $\mathbb{C}^n$. Identify the $n$ data points with the standard basis vectors $e_1, e_2, \ldots, e_n$, where $e_j$ corresponds to the target point. Let $\mathbf{1}$ denote the all-ones vector and set

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

Now we ask two questions.

(i) Can we find two unitary matrices $V_0$ and $V_j$, where $V_j$ depends on $j$ while $V_0$ does not, such that for some integer $k$,

$$\left|\langle (V_0 V_j)^k x_0, e_j\rangle\right|$$

is very close to 1?

(ii) If the above is true, what is $k$?

Grover's search [39] answers both questions—take

$$V_0 = \frac{2}{n}J - I, \quad V_j = 2E_{jj} - I,$$

and then $k$ is an integer closest to $\sqrt{n}$. Here $E_{jj}$ denotes the matrix with 1 in the $jj$-entry and 0 elsewhere.

A Hermitian matrix that is an involution is called a *reflection*. In Grover's search, the first matrix $V_0$ is a reflection about the initial vector $x_0$. The second matrix $V_j$, called the *oracle*, is given as a black box; it acts as a reflection about the target vector $e_j$. In other words, alternately reflecting about $e_j$ and then about $x_0$ a number of times maps $x_0$ to $e_j$.

The above process can be implemented on a quantum computer. A *quantum state* is a one-dimensional subspace of $\mathbb{C}^n$, usually represented by a unit vector $x$. We assume the quantum system evolves in discrete-time, according to a unitary matrix $U$, called the *transition matrix*. More precisely, at step $k$, the system would be in state

$$x_k := U^k x_0,$$

were it in state $x_0$ at time 0. A *measurement* is associated with an $n \times n$ Hermitian matrix $H$, which has real eigenvalues $\{\theta_1, \theta_2, \dots, \theta_n\}$ and an orthonormal basis of eigenvectors $\{v_1, v_2, \dots, v_n\}$. If we measure the system at time $k$, the *outcome* is $\theta_i$ with probability $|\langle x_k, v_i \rangle|^2$. We usually avoid bringing in $H$ by assuming it has simple eigenvalues—in this way, an orthonormal basis of $\mathbb{C}^n$ is sufficient to describe a measurement. Note that every state $x$ can be written as a linear combination of this basis:

$$x = \alpha_1 v_1 + \cdots + \alpha_n v_n.$$

The coefficients $\alpha_1, \alpha_2, \dots, \alpha_n$ are called the *amplitudes*. If more than one amplitude is non-zero, then $x$ is said to be in a *superposition*; in particular,

$$\frac{1}{\sqrt{n}} v_1 + \cdots + \frac{1}{\sqrt{n}} v_n$$

is called the *uniform superposition*.

Now we are ready to describe Grover's search algorithm.

(i) Initialize the system to a uniform superposition of $\{e_1, e_2, \dots, e_n\}$, that is,

$$\frac{1}{\sqrt{n}} e_1 + \cdots + \frac{1}{\sqrt{n}} e_n.$$

(ii) Apply the unitary gate $V_0 V_j$ roughly $\sqrt{n}$ times.

(iii) Measure in the standard basis.

With high probability, the outcome is the target state $e_j$.

This algorithm can also be seen as a quantum walk on a graph. The following observation is due to Ambainis, Kempe and Rivosh [5]. Consider the vector space $\mathbb{C}^n \otimes \mathbb{C}^n$. Let $R$ be the permutation operator that swaps $e_i \otimes e_j$ with $e_j \otimes e_i$ for each $1 \leq i \leq j \leq n$. Then

$$R(V_j \otimes V_0)R = V_0 \otimes V_j.$$

It is not hard to see that for any integer $k$,

$$(R(V_j \otimes V_0))^{2k} = (V_0V_j)^k \otimes (V_jV_0)^k.$$

Thus, the action

$$U := R(V_j \otimes V_0)$$

on $\mathbb{C}^n \otimes \mathbb{C}^n$ is completely determined by the actions of $V_0V_j$ and $V_jV_0$ on $\mathbb{C}^n$. To be more specific, if we start with the uniform superposition

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

then

$$U^k(x_0 \otimes x_0) \approx e_j \otimes \left((V_jV_0)^k x_0\right).$$

Now measuring the first register at step $k$ yields $e_j$ with high probability.

On the other hand, $U$ defines a quantum walk on $X$, the complete graph on $n$ vertices with a loop at each vertex. The state space $\mathbb{C}^n \otimes \mathbb{C}^n$ is spanned by the characteristic vectors $e_u \otimes e_v$ of the arcs $(u, v)$ of $X$. Thus, each state can be seen as a complex-valued function on the arcs of $X$. As an example, the initial state in Grover's search is

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

the constant function that maps each arc to $\frac{1}{n}$. Since $U$ acts linearly on $\mathbb{C}^n \otimes \mathbb{C}^n$, it suffices to investigate its effect on the basis

$$\{e_u \otimes e_v : u \sim v\}.$$

The matrix

$$V_j \otimes V_0 = (2E_{jj} - I) \otimes \left(\frac{2}{n}J - I\right)$$

is usually referred to as the *coin operator*, for it acts as if one flips a quantum coin to determine which arc to move to, given current position. Since

$$(V_j \otimes V_0)(e_u \otimes e_v) = \begin{cases} e_u \otimes \left(\frac{1}{\sqrt{n}} \sum_{w\sim u} e_w\right), & u \neq j, \\ e_u \otimes \left(-\frac{1}{\sqrt{n}} \sum_{w\sim u} e_w\right), & u = j, \end{cases}$$

the result of a coin flip is some superposition of outgoing arcs of current tail $u$. The matrix $R$ is called the *arc-reversal operator*, as it maps the characteristic vector of $(u, v)$ to the characteristic vector of $(v, u)$. These describe how a quantum walker moves on $X$: in each step, she flips the coin to redistribute her amplitudes over the outgoing arcs, and then reverses all the arcs she is on.

## 2.2 Arc-Reversal Walk

Let's rewrite the unitary matrix of Grover's search as

$$\begin{aligned} U &= R(V_j \otimes V_0) \\ &= R(I \otimes V_0)(V_j \otimes I), \end{aligned}$$

and define

$$U_0 := R(I \otimes V_0), \quad U_j := V_j \otimes I.$$

The first matrix $U_0$ defines a quantum walk on $X$, where the coin operator $I \otimes V_0$ treats all vertices equally. The second matrix $U_j$ makes a difference between the marked and unmarked vertices: on outgoing arcs of $j$, it acts as $-I$, while on other arcs it acts as the identity. We say a quantum walk is *unpertubed* if the coins are identical, and *perturbed* if all but one coin are identical. Thus, Grover's search alternates between the unpertubed walk $U_0$ and the oracle operator $U_j$.

The main focus of this thesis will be the unperturbed quantum walk on a general graph. This was first studied by Watrous [62], and later formalized by Kendon [46]. Let $X$ be a $d$-regular graph on $n$ vertices. Consider the space $\mathbb{C}^n \otimes \mathbb{C}^d$ spanned by all complex functions on the arcs of $X$. To each vertex we assign the same *Grover coin*

$$G := \frac{2}{d}J - I.$$

Thus for vertex $u$, the amplitude transfered between two outgoings arcs of $u$ is $2/d - 1$ if they are equal, and $2/d$ otherwise. The coin matrix, acting on $\mathbb{C}^n \otimes \mathbb{C}^d$, is then a direct sum of $n$ Grover coins. Since $G$ commutes with all permutations, we can write the coin matrix as $I \otimes G$ under any basis of $\mathbb{C}^n \otimes \mathbb{C}^d$. Let $R$ be the matrix that reverses all arcs, and set

$$U := R(I \otimes G).$$

The quantum walk with $U$ as the transition matrix is an *arc-reversal walk* on $X$.

It is not hard to extend this definition to a irregular graph: simply assign the Grover coin with $d = \deg(u)$ to vertex $u$. Sometimes we may reconsider the perturbed version as well: give $-G$ to a special vertex and $G$ to the others. More flexibly, any $\deg(u) \times \deg(u)$ unitary matrix $C_u$ could serve as a coin for vertex $u$. However, at this level of generality we will have to specify a linear order on the neighbors of $u$:

$$f_u : \{1, 2, \cdots, \deg(u)\} \to \{v : u \sim v\},$$

in order to define the quantum walk. The vertex $f_u(j)$ will be referred to as the $j$-th neighbor of $u$, and the arc $(u, f_u(j))$ $j$-th arc of $u$. Now we can interpret what $C_u$ does: it sends the $j$-th arc of $u$ to a superposition of all outgoing arcs of $u$, in which the amplitudes come from the $j$-th column of $C_u$:

$$C_u e_j = \sum_{k=1}^{\deg(u)} (e_k^T C_u e_j) e_k.$$

Thus, given that the rows and columns are ordered according to

$$\{f_u : f \in V(X)\},$$

the transition matrix of our quantum walk is

$$U = R \begin{pmatrix} C_1 & & & \\ & C_2 & & \\ & & \ddots & \\ & & & C_n \end{pmatrix}.$$

We sometimes refer to a walk with transition matrix

$$U = R(I \otimes C)$$

an an *arc-reversal $C$-walk*. For an example of this type, see Godsil and Zhan [37].

## 2.3 Two Reflections

There are two major differences of a quantum walk from a classical random walk: first, the evolution is unitary rather than stochastic; second, the transition matrix $U$ does not depend on the graph $X$ only, but also on the coins. In general little can be said about the relation between $U$ and $X$. However, the situation for an arc-reversal walk is a bit special, as its transition matrix $U$ is a product of two reflections related to the graph $X$.

In this section, we develop some machinery that applies to any unitary matrix $U$ as a product of two reflections. Most of the theory here is based on Godsil's unpublished notes [29]. A complete characterization of the eigenvalues and eigenspaces of $U$ is given, by "lifting" those of a smaller Hermitian matrix constructed from the two reflections. This extends Szegedy's work on direct quantization of Markov chains [59]. Our results on the dimensions and structures of the eigenspaces of $U$ will be applied to a different model in Chapter 5.

Let $P$ and $Q$ be two projections acting on $\mathbb{C}^m$. Define

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

Then $U$ lives in the matrix algebra generated by $P$ and $Q$, denoted $\langle P, Q\rangle$. We will use the following well-known fact to diagonalize $U$; a proof by Godsil [29] is provided.

**2.3.1 Lemma.** *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.*

*Proof.* Since $P$ and $Q$ are Hermitian, a subspace of $\mathbb{C}^m$ is $\langle P, Q\rangle$-invariant if and only if its orthogonal complement is $\langle P, Q\rangle$-invariant. Hence $\mathbb{C}^m$ can be decomposed into a direct sum of $\langle P, Q\rangle$-invariant subspaces. Let $W$ be one such subspace.

If $\dim(W) = 1$, then $W$ is spanned by common eigenvectors of $P$ and $Q$, and we are done. So assume $\dim(W) \geq 2$. Since $QPQ$ is also Hermitian, $W$ is a direct sum of eigenspaces for $QPQ$. Depending on how $QPQ$ acts on $W$, we have two cases. Suppose first that $QPQ$ is not zero on $W$. Then there is $z \in \mathbb{C}^m$ and $\mu \neq 0$ such that

$$QPQz = \mu z.$$

Since

$$\mu Qz = Q(QPQ)z = QPQz = \mu z,$$

the vector $z$ must be an eigenvector for $Q$ as well, so

$$Qz = z,$$

and

$$QPz = QPQz = \mu z.$$

It follows that the subspace spanned by $\{z, Pz\}$ is $\langle P, Q\rangle$-invariant. Now suppose $QPQ$ is zero on $W$. If $Q$ is also zero on $W$, then $PQ$ commutes with $QP$ on $W$, and so $W$ is spanned by common eigenvectors of $P$ and $Q$. If $Q$ is not zero on $W$, then it has an eigenvector $z \in W$ with non-zero eigenvalue, that is,

$$Qz = z.$$

Since

$$QPz = QPQz = 0,$$

the subspace spanned by $\{z, Pz\}$ is $\langle P, Q\rangle$-invariant. □

Therefore, to find the spectral decomposition of $U$, we may first decompose $\mathbb{C}^m$ into a direct sum of 1- and 2-dimensional $\langle P, Q\rangle$-invariant subspaces, and then diagonalize $U$ restricted to each of them. The 1-dimensional $\langle P, Q\rangle$-invariant subspaces are precisely common eigenvectors of $P$ and $Q$. In fact, they span the eigenspaces for $U$ with real eigenvalues, that is, 1 and $-1$.

**2.3.2 Lemma.** *Let $P$ and $Q$ be two projections on $\mathbb{C}^m$. Let*

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

*The 1-eigenspace for $U$ is the direct sum*

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

*and the $(-1)$-eigenspace for $U$ is the direct sum*

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

*Proof.* We prove the first statement. The second statement follows by replacing $Q$ with $I - Q$.

If $z$ is in $\mathrm{col}(P) \cap \mathrm{col}(Q)$, then $Pz = z$ and $Qz = z$, so

$$Uy = (2P - I)(2Q - I)y = y.$$

If $z$ is in $\ker(P) \cap \ker(Q)$, then $Pz = 0$ and $Qz = 0$, so

$$Uz = (2P - I)(2Q - I)y = -(-y) = y.$$

By linearity, every vector in

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

is an eigenvector for $U$ with eigenvalue 1. Now suppose $Uz = z$ for some $z \in \mathbb{C}^m$. Then

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

Thus $Pz = Qz$ and $(I - P)z = (I - Q)z$. From the decomposition

$$z = Pz + (I - P)z,$$

we see that $z$ lies in

$$(\operatorname{col}(P) \cap \operatorname{col}(Q)) \oplus (\ker(P) \cap \ker(Q)). \qquad \square$$

It remains to construct eigenvectors for $U$ with non-real eigenvalues. As indicated in the proof of Lemma 2.3.1, the eigenspaces of $PQP$ play a crucial rule in providing the 2-dimensional $U$-invariant subspaces. In practice, we will work with the eigenspaces of a smaller Hermitian matrix that is related to $PQP$, as we describe now.

Being positive-semidefinite, $Q$ has Cholesky decomposition

$$Q = LL^*$$

for some rectangular matrix $L$ with orthonormal columns. Note that

$$QPQz = \mu z$$

if and only if

$$L^*PL(L^*z) = \mu(L^*z).$$

Consequently, for any $\mu \neq 0$, the map $z \mapsto L^*z$ is an isomorphism from the $\mu$-eigenspace of $QPQ$ to the $\mu$-eigenspace of $L^*PL$, with inverse given by $y \mapsto Ly$. We claim that the eigenspaces for $L^*PL$ with non-zero eigenvalues provide all eigenvectors for $U$ with non-real eigenvalues. Our proof uses the following standard result on eigenvalue interlacing; for a reference, see Horn and Johnson [41, Ch 4].

**2.3.3 Theorem.** *Let $A$ be a Hermitian matrix. Let $L$ be a matrix with $L^*L = I$. Let $B = L^*AL$. Then the eigenvalues of $B$ interlace those of $A$.* $\square$

**2.3.4 Lemma.** *Let $P$ and $Q$ be projections on $\mathbb{C}^m$. Let*

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

*Suppose $Q$ has Cholesky decomposition $Q = LL^*$ for some matrix $L$ 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*

$$z \in \operatorname{col}(P) \cap \operatorname{col}(Q).$$

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

$$z \in \ker(P) \cap \operatorname{col}(Q).$$

*(iii) If $y$ 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*

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

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

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

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

*Proof.* Since the columns of $L$ are orthonormal, the eigenvalues of $L^*PL$ interlace those of $P$, which are 0 and 1. If

$$L^*PLy = y,$$

then

$$yL^*(I - P)Ly = 0,$$

and it follows from the positive-definiteness of $I - P$ that $Ly \in \operatorname{col}(P)$. Similarly, if

$$L^*PLy = 0,$$

then $Ly \in \ker(P)$.

Finally, suppose

$$L^*PLy = \mu y$$

for some $\mu \in (0,1)$. Then the subspace spanned by $\{z, Pz\}$ is $U$-invariant:

$$U\begin{pmatrix} z & Pz \end{pmatrix} = \begin{pmatrix} z & Pz \end{pmatrix}\begin{pmatrix} -1 & -2\mu \\ 2 & 4\mu - 1 \end{pmatrix}.$$

To find linear combinations of $z$ and $Pz$ that are eigenvectors of $U$, we diagonalize the matrix

$$\begin{pmatrix} -1 & -2\mu \\ 2 & 4\mu - 1 \end{pmatrix}.$$

It has two eigenvalues: $e^{i\theta}$ with eigenvector

$$\begin{pmatrix} -\cos(\theta) - 1 \\ e^{i\theta} + 1 \end{pmatrix},$$

and $e^{-i\theta}$ with eigenvector

$$\begin{pmatrix} -\cos(\theta) - 1 \\ e^{-i\theta} + 1 \end{pmatrix}.$$

Since $0 < \mu < 1$, these two eigenvalues are distinct, and

$$\frac{\cos(\theta) + 1}{e^{\pm i\theta} + 1} I - P$$

is invertible, so

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

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

The above construction preserves orthogonality—eigenvectors for $U$ obtained from orthogonal eigenvectors for $L^*PL$ are also orthogonal. In the rest of this section, we summarize information on all eigenspaces for $U$ we have seen so far, including their multiplicities. As a consequence, their direct sum is precisely $\mathbb{C}^m$. These results can be found in Zhan [66, 67].

Let

$$P = KK^*$$

for some matrix $K$ with orthonormal columns. Define

$$S := L^*K.$$

This matrix largely determines the spectrum of $U$.

**2.3.5 Lemma.** *Let $P$ and $Q$ be projections on $\mathbb{C}^m$. Let*

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

*The* 1*-eigenspace of $U$ is the direct sum*

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

*which has dimension*

$$m - \mathrm{rk}(P) - \mathrm{rk}(Q) + 2\dim(\mathrm{col}(P) \cap \mathrm{col}(Q)).$$

*Moreover, if*

$$P = KK^*, \quad Q = LL^*$$

*are the Cholesky decompositions of $P$ and $Q$, and*

$$S = L^*K,$$

*then the map $y \mapsto Ly$ is an isomorphism from the* 1*-eigenspace of $SS^*$ to* $\mathrm{col}(P) \cap \mathrm{col}(Q)$.

*Proof.* For the multiplicity, note that

$$\begin{aligned} \dim(\ker(P) \cap \ker(Q)) &= \dim\left(\ker\begin{pmatrix} P \\ Q \end{pmatrix}\right) \\ &= m - \mathrm{rk}\begin{pmatrix} P & Q \end{pmatrix} \\ &= m - \dim(\mathrm{col}\begin{pmatrix} P & Q \end{pmatrix}) \\ &= m - \dim(\mathrm{col}(P) + \mathrm{col}(Q)) \\ &= m - (\mathrm{rk}(P) + \mathrm{rk}(Q) - \dim(\mathrm{col}(P) \cap \mathrm{col}(Q))). \end{aligned}$$

The isomorphism follows from Lemma 2.3.4 and the previous discussion. □

**2.3.6 Lemma.** *Let $P$ and $Q$ be projections on $\mathbb{C}^m$, with Cholesky decompositions*

$$P = KK^*, \quad Q = LL^*.$$

*Let*

$$S = L^*K.$$

*Let*

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

*The $(-1)$-eigenspace of $U$ is the direct sum*

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

*which has dimension*

$$\mathrm{rk}(P) + \mathrm{rk}(Q) - 2\,\mathrm{rk}(S).$$

*Moreover, the map $y \mapsto Ky$ is an isomorphism from $\ker(S)$ to $\mathrm{col}(P)\cap\ker(Q)$, and the map $y \mapsto L^*y$ is an isomorphism from $\ker(S^*)$ to $\ker(P) \cap \mathrm{col}(Q)$.*

*Proof.* We prove the last part of the statement, from which the dimension follows. If

$$Sy = 0,$$

then

$$QKy = LSy = 0.$$

Hence

$$Ky \in \mathrm{col}(P) \cap \ker(Q).$$

Further, since $K$ has full column rank, this map is injective. On the other hand, for any $z \in \mathrm{col}(P) \cap \ker(Q)$, there is some $y$ such that

$$z = Ky$$

and

$$0 = Qz = LSy = L^*LSy = Sy,$$

which implies that

$$y \in \ker(S).$$

The argument for the second linear map is similar. □

**2.3.7 Lemma.** *Let $P$ and $Q$ be projections on $\mathbb{C}^m$, with Cholesky decompositions*

$$P = KK^*, \quad Q = LL^*.$$

*Let*

$$S = L^*K.$$

*Let*

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

*The dimensions of the eigenspaces for $U$ with non-real eigenvalues sum to*

$$2\,\mathrm{rk}(S) - 2\dim(\mathrm{col}(P) \cap \mathrm{col}(Q)).$$

*Let $\mu \in (0,1)$ be an eigenvalue of $SS^*$. Let $\theta$ be such that $\cos(\theta) = 2\mu - 1$. The map*

$$y \mapsto ((\cos(\theta) + 1)I - (e^{i\theta} + 1)P)Ly$$

*is an isomorphism from the $\mu$-eigenspace of $SS^*$ to the $e^{i\theta}$-eigenspace of $U$, and the map*

$$y \mapsto ((\cos(\theta) + 1)I - (e^{-i\theta} + 1)P)Ly$$

*is an isomorphism from the $\mu$-eigenspace of $SS^*$ to the $e^{-i\theta}$-eigenspace of $U$.*

*Proof.* By Lemma 2.3.4 and Lemma 2.3.5, the eigenspaces for $SS^*$ with eigenvalues in $(0,1)$ provide

$$2(\mathrm{rk}(SS^*) - \dim(\mathrm{col}(P) \cap \mathrm{col}(Q)))$$

orthogonal eigenvectors for $U$. Combining this with Lemma 2.3.6, we see that they span the orthogonal complement of the $(\pm 1)$-eigenspaces. The isomophisms now follow from Lemma 2.3.4. □

For normalization purpose, note that

$$\left\|((\cos(\theta) + 1) - (e^{\pm i\theta} + 1)P)Ly\right\|^2 = \sin^2(\theta)(\cos(\theta) + 1)\|y\|^2.$$

This will become useful when we compute the orthogonal projection onto the $e^{\pm i\theta}$-eigenspace.

With the theory developed in this section, we can derive the spectral decomposition of any matrix in the algebra generated by $P$ and $Q$. By comparison, Szegedy [59] computed the eigenvalues and eigenvectors specifically for the matrix $(2P - I)(2Q - I)$.

## 2.4 Graph Spectra vs Walk Spectra

Let $X$ be a connected $d$-regular graph on $n$ vertices, and $U$ the transition matrix of the arc-reversal walk on $X$. In this section, we show that the spectrum of $X$ determines the spectrum of $U$. More specifically, eigenvalues of $X$ provide the real parts of eigenvalues of $U$, and eigenvectors of $X$ can be lifted to eigenvectors of $U$ by two incidence matrices. Most of the results below can be found in Zhan [66].

Recall that

$$U = R(I \otimes G),$$

where $R$ is the arc-reversal matrix, and $G$ the $d \times d$ Grover coin. Since

$$R^2 = (I \otimes G)^2 = I,$$

all observations in the previous section apply. To see what $R$ and $I \otimes G$ reflect about, we introduce four incidence matrices: the tail-arc incidence matrix $D_t$, the head-arc incidence matrix $D_h$, the arc-edge incidence matrix $M$, and the vertex-edge incidence matrix $B$.

The tail-arc incidence matrix $D_t$, and the head-arc incidence matrix $D_h$, are two matrices with rows indexed by the vertices, and columns by the arcs. If $u$ is a vertex and $a$ is an arc, then $(D_t)_{u,a} = 1$ if $u$ is the initial vertex of $a$, and $(D_h)_{u,a} = 1$ if $a$ ends on $u$, and 0 otherwise.

The arc-edge incidence matrix $M$ is a matrix with rows indexed by the arcs and columns by the edges. If $a$ is an arc and $e$ is an edge, then $M_{a,e} = 1$ if $a$ is one direction of $e$, and 0 otherwise.

The vertex-edge incidence matrix $B$ is a matrix with rows indexed by the vertices and columns by the edges. If $u$ is a vertex and $e$ is an edge, then $B_{u,e} = 1$ if $u$ is one endpoints of $e$, and 0 otherwise.

As an example, the following are the four incidence matrices associated with $K_3$ with vertices $\{0, 1, 2\}$.

$$D_t = \begin{array}{c} \\ 0 \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cccccc} (0,1) & (0,2) & (1,0) & (1,2) & (2,0) & (2,1) \end{array} \\ \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 \end{pmatrix} \end{array}$$

$$D_h = \begin{array}{c} \\ 0 \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{cccccc} (0,1) & (0,2) & (1,0) & (1,2) & (2,0) & (2,1) \end{array} \\ \begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 0 \end{pmatrix} \end{array}$$

$$M = \begin{array}{c} \\ (0,1) \\ (0,2) \\ (1,0) \\ (1,2) \\ (2,0) \\ (2,1) \end{array} \begin{array}{c} \begin{array}{ccc} \{0,1\} & \{0,2\} & \{1,2\} \end{array} \\ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \end{array}$$

$$B = \begin{array}{c} \\ 0 \\ 1 \\ 2 \end{array} \begin{array}{c} \begin{array}{ccc} \{0,1\} & \{0,2\} & \{1,2\} \end{array} \\ \begin{pmatrix} 1 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix} \end{array}$$

Next, we list some useful identities about these incidence matrices.

**2.4.1 Lemma.** *Let $X$ be a $d$-regular graph. Let $A$ be the adjacency matrix of $X$. Let $D_t$ and $D_h$ be the tail-arc incidence matrix and the head-arc incidence matrix, respectively. Let $M$ be the arc-edge incidence matrix. Let $B$ be the vertex-edge incidence matrix. Let $G$ be the $d \times d$ Grover coin. The following identities hold.*

(i) $D_t^T D_t = D_h^T D_h = dI$.

(ii) $M^T M = 2I$.

(iii) $D_t D_h^T = D_h D_t^T = A$.

(iv) $BB^T = A + dI$.

(v) $D_t M = D_h M = B$.

(vi) $D_t R = D_h$.

(vii) $R = MM^T - I$.

(viii) $I \otimes G = \frac{2}{d} D_t^T D_t - I \otimes I$.

*Proof.* We give a proof for (iii). Let $u$ and $v$ be two vertices of $X$. We have

$$\begin{aligned}(D_t D_h^T)_{uv} &= \langle D_t^T e_u, D_h^T e_v \rangle \\ &= |\{(a,b) : \{a,b\} \in E(X), a = u, b = v\}|\end{aligned}$$

$$= \begin{cases} 1, & \{u,v\} \in E(X) \\ 0, & \{u,v\} \notin E(X). \end{cases}$$

Therefore $D_t D_h^T = A$. Since $A$ is symmetric, we also have $D_h D_t^T = A$. The remaining identities can be verified in a similar manner. □

As a consequence, $R$ is a reflection about $\operatorname{col}(M)$, while $I \otimes G$ is a reflection about $\operatorname{col}(D_t^T)$. We now prove the spectral relation between $U$ and $A$. The following theorem shows that all eigenspaces of $U$ with non-real eigenvalues are completely determined by the eigenspaces of $X$ with eigenvalues in $(-d, d)$. It also gives a concrete description on how to "lift" eigenvalues and eigenvectors of $X$ to those of $U$.

**2.4.2 Theorem.** *Let $X$ be a $d$-regular graph. Let $D_t$ and $D_h$ be the tail-arc incidence matrix and the head-arc incidence matrix, respectively. Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. The multiplicities of the non-real eigenvalues of $U$ sum to $2n-4$ if $X$ is bipartite, and $2n-2$ otherwise. Let $y$ be an eigenvector for $X$ with eigenvalue $\lambda \in (-d, d)$. Let $\theta \in \mathbb{R}$ be such that $\lambda = d\cos(\theta)$. Then*

$$D_t^T y - e^{i\theta} D_h^T y$$

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

$$D_t^T y - e^{-i\theta} D_h^T y$$

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

*Proof.* Let

$$K := \frac{1}{\sqrt{2}} M, \quad L := \frac{1}{\sqrt{d}} D_t^T, \quad S := L^* K.$$

Let $B$ be the vertex-edge incidence matrix of $X$. According to Lemma 2.3.7, the eigenspaces for $U$ with non-real eigenvalues are determined by eigenspaces for

$$SS^* = \frac{1}{2d} BB^T = \frac{1}{2d}(A + dI).$$

Let

$$\mu := \frac{\lambda + d}{2d}.$$

Then $0 < \mu < 1$ and $2\mu - 1 = \cos(\theta)$. Moreover,

$$Ay = \lambda y$$

if and only if

$$SS^* y = \mu y.$$

Thus, using identities in Lemma 2.4.1, we obtain two eigenvectors for $U$ as stated. □

After normalization, we obtain the eigenprojections for non-real eigenvalues of $U$.

**2.4.3 Corollary.** *Let $X$ be a $d$-regular graph. Let $D_t$ and $D_h$ be the tail-arc incidence matrix and the head-arc incidence matrix, respectively. Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. Let $\lambda$ be an eigenvalue of $X$ that is neither $d$ nor $-d$. Let $E_\lambda$ be the orthogonal projection onto the $\lambda$-eigenspace of $X$. Suppose $\lambda = d\cos(\theta)$ for some $\theta \in \mathbb{R}$. Then the $e^{i\theta}$-eigenprojection of $U$ is*

$$\frac{1}{2d\sin^2(\theta)}(D_t - e^{i\theta} D_h)^T E_\lambda (D_t - e^{-i\theta} D_h),$$

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

$$\frac{1}{2d\sin^2(\theta)}(D_t - e^{-i\theta} D_h)^T E_\lambda (D_t - e^{i\theta} D_h). \qquad \square$$

We also characterize the $(\pm 1)$-eigenspaces of $U$. In particular, their multiplicities depend on parameters of $X$.

**2.4.4 Lemma.** *Let $X$ be a $d$-regular graph. Let $D_t$ be the tail-arc incidence matrix. Let $M$ be the arc-edge incidence matrix. Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. The 1-eigenspace of $U$ is*

$$(\operatorname{col}(M) \cap \operatorname{col}(D_t^T)) \oplus (\ker(M^T) \cap \ker(D_t))$$

*with dimension*

$$\frac{nd}{2} - n + 2.$$

*Moreover, the projection onto $\operatorname{col}(M) \cap \operatorname{col}(D_t^T)$ is given by*

$$\frac{1}{d} D_t^T E_d D_t = \frac{1}{nd} J,$$

*where $E_d$ is the projection onto the $d$-eigenspace of $X$.*

*Proof.* By Lemma 2.3.5, the 1-eigenspace is the direct sum:

$$(\operatorname{col}(M) \cap \operatorname{col}(D_t^T)) \oplus (\ker(M^T) \cap \ker(D_t)),$$

where

$$\operatorname{col}(M) \cap \operatorname{col}(D_t^T) = D_t \operatorname{col}(E_d).$$

Note that $\operatorname{col}(D_t^T)$ consists of vectors that are constant over the outgoing arcs of each vertex, and $\operatorname{col}(M)$ consists of vectors that are constant over each pair of opposite arcs. Since $X$ is connected,

$$\operatorname{col}(M) \cap \operatorname{col}(D_t^T) = \operatorname{span}\{\mathbf{1}\}.$$

The multiplicity follows from the fact that $\operatorname{rk}(M) = nd/2$ and $\operatorname{rk}(D_t) = n$. □

**2.4.5 Lemma.** *Let $X$ be a $d$-regular graph. Let $D_t$ be the tail-arc incidence matrix. Let $M$ be the arc-edge incidence matrix. Let $B$ be the vertex-edge incidence matrix. Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. If $X$ is bipartite, the $(-1)$-eigenspace of $U$ is*

$$M \ker(B) \oplus D_t^T \ker(B^T)$$

*with dimension*

$$\frac{nd}{2} - n + 2.$$

*Moreover, the projection onto $D_t^T \ker(B^T)$ is given by*

$$\frac{1}{d} D_t^T E_{-d} D_t,$$

*where $E_{-d}$ is the projection onto the $(-d)$-eigenspace of $X$. If $X$ is not bipartite, the $(-1)$-eigenspace of $U$ is*

$$M \ker(B),$$

*with dimension*

$$\frac{nd}{2} - n.$$

*Proof.* By Lemma 2.3.6, the $(-1)$-eigenspace of $U$ is

$$M \ker(B) \oplus D_t^T \ker(B^T),$$

where

$$\ker(B^T) = \operatorname{col}(E_{-d}).$$

Note that $\operatorname{rk}(B) = n - 1$ if $X$ is bipartite, and $\operatorname{rk}(B) = n$ otherwise. □

The spectra of variants of $U$ are also of interest for producing graph isomorphism algorithms. In [21, 22], Emms, Severini, Wilson and Hancock proposed a scheme to distinguish non-isomorphic graphs, based on the spectrum of the positive support of $U^3$. Godsil and Guo [31] then studied the relation between the spectra of positive supports of $U$, $U^2$ and $U^3$ in greater detail. Later in [32], Godsil, Guo and Myklebust found two non-isomorphic strongly regular graphs whose positive supports of $U^3$ have the same spectrum.

## 2.5 Perfect State Transfer

Both continuous and discrete quantum walks were shown to be universal for quantum computation [16, 52, 60]. An important ingredient, in implementing the universal quantum gates using quantum walks, is perfect state transfer. Loosely speaking, a graph admits perfect state transfer from vertex $u$ to vertex $v$ if for some real number $t$, measuring the system at step $t$ yields vertex $v$ with certainty, given that the system "concentrated" on vertex $u$ at the beginning. For discrete quantum walks, this is equivalent to requiring the initial state to be a superposition over the outgoing arcs of $u$, and the final state to be a superposition over the outgoing arcs of $v$. Sometimes there are more restrictions on the initial and final states; we will give a formal definition later.

While there have been numerous results on perfect state transfer in continuous quantum walks [7, 8, 9, 14, 18, 19, 20, 42, 43, 47], less is known on the discrete side, as the extra coins make it harder to analyze the transition operator. Most of the examples in discrete quantum walks were sporadic, and there was no infinite family of $k$-regular graphs with perfect state transfer, for any $k \geq 3$. Kurzynski and Wojcik [49] showed that perfect state transfer on cycles can be achieved in discrete quantum walks. In their paper, they also discussed how to convert the position dependence of couplings into the position dependence of coins. Barr, Proctor, Allen, and Kendon[11] investigated discrete quantum walks on variants of cycles, and found some families that admit perfect state transfer with appropriately chosen coins and initial states. In [64], Yalcnkaya and Gedik proposed a scheme to achieve perfect state transfer on paths and cycles using a recovery operator. With various setting of coin flippings, Xiang Zhan et al [68] also showed that an arbitrary unknown two-qubit state can be perfectly transfered in one-dimensional or two-dimensional lattices. Recently, Stefanak and Skoupy analyzed perfect state transfer in perturbed quantum walks on stars [57] and complete bipartite graphs [58] between marked vertices: in $K_{n,n}$, perfect state transfer occurs between any two marked vertices, while in $K_{m,n}$ with $m \neq n$, perfect state transfer only occurs between two marked vertices on the same side.

In this section, we derive necessary and sufficient conditions for perfect state transfer to occur. The techniques we use are very similar to those employed in continuous quantum walks. For a thorough treatment of continuous-time perfect state transfer, see Coutinho's Ph.D. thesis [17]. Although the transition matrix $U$ is not an obvious function of the adjacency matrix $A$ of the graph, we show that perfect state transfer can be characterized purely in terms of $A$. Using our characterization, we provide the first infinite family of graphs, other than variants of cycles, that admit antipodal perfect state transfer in unperturbed discrete quantum walks. These are circulant graphs whose connection sets satisfy a simple condition.

Let $X$ be a $d$-regular graph on $n$ vertices. An arc-reversal quantum walk takes place in $\mathbb{C}^n \otimes \mathbb{C}^d$. Suppose we start with a state that "concentrates on" $u$. In theory, this could be $e_u \otimes x$ for any unit vector $x$. However, it is more practical to prepare a uniform superposition over the outgoing arcs of $u$:

$$\frac{1}{\sqrt{d}} e_u \otimes \mathbf{1}.$$

Formally, if there is a unit vector $x \in \mathbb{C}^d$ such that

$$U^k \left( \frac{1}{\sqrt{d}} e_u \otimes \mathbf{1} \right) = e_v \otimes x,$$

then we say $X$ admits *perfect state transfer* from $u$ to $v$ if $u \neq v$, and $X$ is *periodic* at $u$ if $u = v$. While this definition does not impose further condition on the final state, in the arc-reversal walk, the only possible choice of $x$ is

$$\frac{1}{\sqrt{d}} \mathbf{1},$$

as we show now.

**2.5.1 Lemma.** *Let $X$ be a regular graph. Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. If $X$ admits perfect state transfer from $u$ to $v$ at time $k$, then*

$$U^k \left( \frac{1}{\sqrt{d}} e_u \otimes \mathbf{1} \right) = \frac{1}{\sqrt{d}} e_v \otimes \mathbf{1}.$$

*Proof.* Suppose
$$U^k\left(\frac{1}{\sqrt{d}}e_u \otimes \mathbf{1}\right) = e_v \otimes x.$$
Since $U$ has real entries, all entries in $x$ are also real. Moreover, as $\mathbf{1}\otimes\mathbf{1}$ is an eigenvector for $U$ with eigenvalue 1,
$$\left\langle \mathbf{1}\otimes\mathbf{1}, \frac{1}{\sqrt{d}}e_u \otimes \mathbf{1}\right\rangle = \left\langle \mathbf{1}\otimes\mathbf{1}, U^k\left(\frac{1}{\sqrt{d}}e_u \otimes \mathbf{1}\right)\right\rangle = \langle \mathbf{1}\otimes\mathbf{1}, e_v \otimes x\rangle.$$
If $X$ is $d$-regular, then it follows that
$$\langle \mathbf{1}, x\rangle = \sqrt{d}.$$
On the other hand, by Cauchy-Schwarz,
$$|\langle \mathbf{1}, x\rangle| \leq \|\mathbf{1}\|\|x\| = \sqrt{d},$$
with equality held if and only if $x$ is a scalar multiple of $\mathbf{1}$. Therefore $x$ must be equal to $\mathbf{1}$. □

Notice that both the initial state and the final state lie in $\operatorname{col}(D_t^T)$, so an equivalent definition for perfect state transfer from $u$ to $v$ at time $k$ is
$$U^k D_t^T e_u = D_t^T e_v.$$
Our characterization of perfect state transfer relies heavily on this observation.

**2.5.2 Lemma.** *Let $X$ be a $d$-regular graph. Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. Let $\lambda = d\cos(\theta)$ be an eigenvalue of $X$ that is neither $d$ nor $-d$. Let $E_\lambda$ be the projection onto the $\lambda$-eigenspace of $X$, and let $F_\pm$ be the projection onto the $e^{\pm i\theta}$-eigenspace of $U$. Then*
$$D_t F_\pm D_t^T = \frac{d}{2}E_\lambda.$$

*Proof.* By Lemma 2.4.3,
$$\begin{aligned} 2d\sin^2(\theta) D_t F_\pm D_t^T &= D_t(D_t - e^{\pm i\theta})^T E_\lambda (D_t - e^{\mp i\theta} D_h) \\ &= (dI - e^{\pm i\theta}A)E_\lambda(dI - e^{\mp i\theta}A) \\ &= d^2\left|1 - e^{i\theta}\cos(\theta)\right|^2 E_\lambda \\ &= d^2\sin^2(\theta)E_\lambda. \end{aligned}$$
□

**2.5.3 Theorem.** *Let $X$ be a $d$-regular graph, with spectral decomposition*

$$A = \sum_{\lambda} \lambda E_{\lambda}.$$

*Then the arc-reversal Grover walk on $X$ admits perfect state transfer from $u$ to $v$ at time $k$ if and only if all of the following hold.*

*(i) For each $\lambda$, we have $E_{\lambda} e_u = \pm E_{\lambda} e_v$.*

*(ii) If $E_{\lambda} e_u = E_{\lambda} e_v \neq 0$, then there is an even integer $j$ such that*

$$\lambda = d \cos(j\pi/k).$$

*(iii) If $E_{\lambda} e_u = -E_{\lambda} e_v \neq 0$, then there is an odd integer $j$ such that*

$$\lambda = d \cos(j\pi/k).$$

*Proof.* Let $U$ be the transition matrix of the arc-reversal Grover walk on $X$. Consider the spectral decomposition of $U$:

$$U = \sum_{r} e^{i\theta_r} F_r.$$

There is perfect state transfer from $u$ to $v$ at time $k$ if and only if

$$\sum_{r} e^{ik\theta_r} F_r D_t^T e_u = D_t^T e_v,$$

or equivalently, for each $r$,

$$e^{ik\theta_r} F_r D_t^T e_u = F_r D_t^T e_v. \tag{2.5.1}$$

We prove that Equation (2.5.1) holds if and only if (i), (ii) and (iii) hold. Depending on $r$, there are three cases.

Suppose $e^{i\theta_r} = 1$. Equation (2.5.1) says that

$$F_r D_t^T e_u = F_r D_t^T e_v.$$

By Lemma 2.4.4, this holds if and only if

$$\frac{1}{nd} J e_u = D_t^T E_d e_u = D_t^T E_d e_v = \frac{1}{nd} J e_v \neq 0,$$

if and only if

$$E_d e_u = E_d e_v \neq 0.$$

Clearly $d = d\cos(0)$, which satisfies (ii).

Suppose $e^{i\theta_r} = -1$. By Lemma 2.4.5,

$$F_r D_t^T = \frac{1}{d} D_t^T E_{-d} D_t D_t^T = D_t^T E_d.$$

Thus Equation (2.5.1) holds if and only if

$$(-1)^k F_r D_t^T e_u = F_r D_t^T e_v,$$

that is,

$$(-1)^k D_t^T E_{-d} e_u = D_t^T E_{-d} e_v.$$

If $X$ is not bipartite, then $E_{-d} = 0$ and

$$F_r D_t^T e_u = F_r D_t^T e_v = 0.$$

Otherwise,

$$E_{-d} e_u = E_{-d} e_v \neq 0$$

if $u$ and $v$ are in the same color class, and

$$E_{-d} e_u = -E_{-d} e_v \neq 0$$

if they are in different color classes. Clearly

$$-d = d\cos\left(\frac{k\pi}{k}\right),$$

which satisfies (i) and (ii).

Finally suppose $e^{i\theta_r} \neq \pm 1$. Equation (2.5.1) says that

$$e^{ik\theta_r} F_r D_t^T e_u = F_r D_t^T e_v.$$

By Lemma 2.5.2,

$$D_t F_r D_t^T = \frac{d}{2} E_\lambda,$$

so

$$\frac{de^{ik\theta_r}}{2} (E_\lambda)_{uu} = e^{ik\theta_r} \left\langle F_r D_t^T e_u, D_t^T e_u \right\rangle = \left\langle F_r D_t^T e_v, D_t^T e_u \right\rangle = \frac{d}{2} (E_\lambda)_{uv} \in \mathbb{R}.$$

Therefore Equation (2.5.1) holds if and only if one of the following occurs:

(a) $E_\lambda e_u = E_\lambda e_v = 0$;

(b) $E_\lambda e_u = E_\lambda e_v \neq 0$, and $e^{ik\theta_r} = 1$;

(c) $E_\lambda e_u = -E_\lambda e_v \neq 0$, and $e^{ik\theta_r} = -1$. □

The three conditions in Theorem 2.5.3 are symmetric in $u$ and $v$. As a consequence, perfect state transfer is symmetric in the initial and final state, and it implies periodicity at both vertices.

**2.5.4 Corollary.** *Let $X$ be a regular graph. Consider the arc-reversal Grover walk on $X$. If there is perfect state transfer from $u$ to $v$ at time $k$, then there is perfect state transfer from $v$ to $u$ at time $k$, and $X$ is periodic at both $u$ and $v$ at time $2k$.* □

Let $X$ be a graph with spectral decomposition

$$A = \sum_\lambda \lambda E_\lambda.$$

The *eigenvalue support* of a vertex $u$, defined by Godsil [26], is the set

$$\{\lambda : E_\lambda e_u \neq 0\}.$$

Let $\phi(t)$ be the characteristic polynomial of $X$, and $\phi_u(t)$ the characteristic polynomial of the vertex-deleted subgraph $X\backslash u$. It is shown by Godsil and Royle [34] that the eigenvalue support of $u$ consists of roots of the following polynomial:

$$\psi_u(t) := \frac{\phi(t)}{\gcd(\phi(t), \phi_u(t))}.$$

Thus, Theorem 2.5.3 gives necessary and sufficient conditions on $\psi_u(t)$ for $X$ to be periodic at $u$.

**2.5.5 Theorem.** *Suppose $\psi_u(t)$ has degree $\ell$. Then vertex $u$ is periodic at time $k$ if and only if the polynomial*

$$z^\ell \psi_u\left(\frac{d}{2}\left(z + \frac{1}{z}\right)\right)$$

*is a factor of $z^k - 1$.*

*Proof.* Setting $u = v$ in Theorem 2.5.3, we see that $u$ is periodic at time $k$ if and only if each eigenvalue $\lambda$ in the eigenvalue support of $u$ is of the form

$$\lambda = \frac{d}{2}(e^{j\pi i/k} + e^{-j\pi i/k}),$$

for some even integer $j$, or equivalently,

$$z^{\ell}\psi_u\left(\frac{d}{2}\left(z+\frac{1}{z}\right)\right)$$

divides $z^k - 1$. □

Two vertices $u$ and $v$ in $X$ are *cospectral* if the the vertex-deleted subgraphs $X\backslash u$ and $X\backslash v$ have the same characteristic polynomial, that is,

$$\phi_u(t) = \phi_v(t).$$

We say two vertices $u$ and $v$ are *strongly cospectral* if

$$E_\lambda e_u = \pm E_\lambda e_v$$

for each eigenvalue $\lambda$ of $X$. Strongly cospectrality has been thoroughly studied by Godsil and Smith [35]; we cite a useful characterization below.

**2.5.6 Theorem.** *Let $X$ be a graph with spectral decomposition*

$$A = \sum_\lambda \lambda E_\lambda.$$

*Two vertices $u$ and $v$ in $X$ are strongly cospectral if and only if both*

*(i) $u$ and $v$ are cospectral; and*

*(ii) for every eigenvalue $\lambda$ of $X$, the vectors $E_\lambda e_u$ and $E_\lambda e_v$ are parallel.* □

Conditions (ii) and (iii) in Theorem 2.5.3 lead us to consider regular graphs whose eigenvalues are given by real parts of $2k$-th roots of unity. A *circulant graph* $X = X(\mathbb{Z}_n, \{g_1, g_2, \ldots, g_d\})$ is a Cayley graph over $\mathbb{Z}_n$ with inverse-closed connection set

$$\{g_1, g_2, \ldots, g_d\} \subseteq \mathbb{Z}_n.$$

If $\psi$ is a character of $\mathbb{Z}_n$, then $\psi$ is also an eigenvector for $X$ with eigenvalue

$$\psi(g_1) + \cdots + \psi(g_d).$$

Note that this is a sum of real parts of $n$-th roots of unity. We show that circulant graphs whose connection sets satisfy a simple condition admit perfect state transfer. The following can be found in Zhan [66].

**2.5.7 Theorem.** *Let $\ell$ be an odd integer. For any distinct integers $a$ and $b$ such that $a+b=\ell$, the arc-reversal Grover walk on the circulant graph $X(\mathbb{Z}_{2\ell}, \{a, b, -a, -b\})$ admits perfect state transfer at time $2\ell$ from vertex $0$ to vertex $\ell$.*

*Proof.* The eigenvalues of $X$ are

$$\begin{aligned}\lambda_j &= e^{aj\pi/\ell} + e^{-aj\pi/\ell} + e^{bj\pi/\ell} + e^{-bj\pi/\ell} \\ &= 2\cos\left(\frac{aj\pi}{\ell}\right) + 2\cos\left(\frac{bj\pi}{\ell}\right),\end{aligned}$$

for $j = 0, 1, \cdots, 2n-1$. Since $\ell$ is odd and $a+b=\ell$, when $j$ is odd,

$$\lambda_j = 0 = 4\cos\left(\frac{\ell\pi}{2\ell}\right),$$

and when $j$ is even,

$$\lambda_j = 4\cos\left(\frac{2aj\pi}{2\ell}\right).$$

It suffices to check the parity condition in Theorem 2.5.3 for each eigenvector of $X$. Since $a+b=\ell$, vertex $u$ and $u+\ell$ have the same neighbors, so

$$A(e_u - e_{u+\ell}) = 0.$$

We see from the multiplicity of 0 that for $u = 0, 1, \cdots, \ell-1$, the vectors $e_u - e_{u+\ell}$ form an orthogonal basis for $\ker(A)$. Thus $y_u = -y_v$ if $y$ is an eigenvector for $X$ with eigenvalue 0, and $y_u = y_v$ if $y$ is any other eigenvector for $X$. □

## 2.6 Open Problems

We end this chapter with some open problems on arc-reversal walks.

One obvious direction is to find more examples of perfect state transfer. Since perfect state transfer at step $k$ implies periodicity at step $2k$, the first question we could ask is the following.

(i) Which regular graphs have periodic vertices?

Theorem 2.5.5 gives a characterization for periodic vertices. Although this is a local condition on the eigenvalue support of a vertex, it is satisfied when the entire graph is periodic, that is, when all eigenvalues of the graph are $d$ times the real parts of some $k$-th roots of unity. Hence, it is useful to study graphs for which

$$z^n \phi\left(\frac{d}{2}\left(z+\frac{1}{z}\right)\right)$$

is a factor of $z^k - 1$. In [65], Yoshie investigated periodic arc-reversal Grover walks on distance regular graphs, and found all Hamming graphs and Johnson graphs that are periodic.

Looking back at our definition of perfect state transfer, we see that it is because the initial state lives in $\operatorname{col}(D_t^T)$ that perfect state transfer can be characterized using graph spectra. In theory, for any unit vector $x$,

$$e_u \otimes x$$

could serve as the initial state that concentrates on $u$. Thus, the second question is to understand what happens if we relax the assumption on the initial state.

(ii) Is there an example of perfect state transfer, where the initial state does not lie in $\operatorname{col}(D_t^T)$? If so, can we characterize such perfect state transfer purely in terms of the spectral decomposition of $X$?

Finally, while most of our theory was devoted to arc-reversal Grover walks, there are other coins that have been studied in the literature, such as the Fourier coin:

$$F := \frac{1}{\sqrt{d}}(e^{2jk\pi i/d})_{jk}.$$

Note that $F^4 = I$, so the techniques in Section 2.3 do not apply. However, for graphs with special structures, one can still study the arc-reversal Fourier walk analytically. In [48], Krovi and Brun computed the hitting time of an arc-reversal walk on the hypercube $Q_d$, and showed that for some initial state, the hitting time relative to

$$U = R(I \otimes F)$$

could be infinite. This is in sharp contrast to the polynomial hitting time relative to

$$U = R(I \otimes G),$$

as proved by Kempe [45]. Below we give another example showing how coins may affect the behavior of a quantum walk.

**2.6.1 Theorem.** *Let $X = K_{m,n}$. For each vertex $u$, let $f_u$ be a linear order on its neighbors. Suppose $f_u = f_v$ whenever $u$ and $v$ are in the same color class. Let $C_n$ be an $m \times m$ unitary coin of order $k$, and attach it to each vertex of degree $n$. Let $C_m$ an $n \times n$ unitary coin of order $\ell$, and attach it to each vertex of degree $m$. If $U$ is the transition matrix of the arc-reversal walk on $X$ with coins $C_m$ and $C_n$, then*

$$U^{2\operatorname{lcm}(k,\ell)} = I.$$

*Proof.* Up to permuting the row and the columns, the transition matrix can be written as

$$U = R \begin{pmatrix} C_n & & & & & \\ & \ddots & & & & \\ & & C_n & & & \\ & & & C_m & & \\ & & & & \ddots & \\ & & & & & C_m \end{pmatrix},$$

where

$$R = E_{12} \otimes \left( \sum_{i=1}^{m} \sum_{j=1}^{n} E_{ji} \otimes E_{ij} \right) + E_{21} \otimes \left( \sum_{i=1}^{m} \sum_{j=1}^{n} E_{ij} \otimes E_{ji} \right).$$

Thus,

$$U = R(E_{11} \otimes I_m \otimes C_n + E_{22} \otimes I_n \otimes C_m)$$

$$= E_{12} \otimes \left( \sum_{i=1}^{m} \sum_{j=1}^{n} E_{ji} \otimes E_{ij} C_m \right) + E_{21} \otimes \left( \sum_{i=1}^{m} \sum_{j=1}^{n} E_{ij} \otimes E_{ji} C_n \right).$$

Therefore,

$$U^2 = E_{11} \otimes \left( \sum_{j=1}^{n} \sum_{t=1}^{m} E_{jt} (C_m)_{jt} \right) \otimes C_n + E_{22} \otimes \left( \sum_{i=1}^{m} \sum_{s=1}^{n} E_{is} (C_n)_{is} \right) \otimes C_m$$
$$= \begin{pmatrix} C_m \otimes C_n & 0 \\ 0 & C_n \otimes C_m \end{pmatrix}.$$

It follows that the order of $U^2$ divides the order of $C_m \otimes C_n$, that is, $\operatorname{lcm}(k, m)$. □

We pose a question about optimizing certain parameter over arc-reversal walks with arbitrary coins, but keep in mind that this may be fairly difficult to solve, so even partial progress will be useful. One interesting parameter of a quantum walk is the mixing time; we will discuss this in Chapter 3.

(iii) Given an important parameter of discrete quantum walks, and an arc-reversal walk with transition matrix

$$U = R(I \otimes C),$$

can we optimize the parameter over all possible coins $C$?

# Chapter 3

# General Quantum Walks

In the last chapter, our quantum walker discovered a simple rule to move on a $d$-regular graph: at each step, she pushes her part on arc $(u, v)$ towards arc $(v, w)$, with "relocation amplitude" $2/d - 1$ if $w$ and $v$ are equal, and $2/d$ otherwise. After exploring for a while, she starts to modify the rule. First, the arc that receives relocation amplitude $2/d - 1$ does not have to be the inverse of the previous one—she could pick the special arc in her own way. Second, these amplitudes do not have to be real—she could toss any complex coin as long as it stays unitary. Finally, the underlying graph does not have to be regular or undirected—she could assign different coins to different vertices based on their outdegrees. However, as time goes, she notices some common phenomena of these quantum walks, due to the nature of unitarity.

The aim of this chapter is to study the limiting behavior of a quantum walk while assuming as little as possible. To allow this level of generality, we suppose the underlying graph $X$ is directed, and $U$ is simply a unitary matrix indexed by the arcs of $X$. We will consider the applications to specific quantum walks in later chapters.

We start by describing the evolution of a quantum walk in the density matrix formalism, as it cleans up the discussion on various forms of probabilities. Following this, we show that while the instantaneous probability distribution of a quantum walk does not converge, its Cesàro sum does exist, and can be expressed using the spectral idempotents of $U$. We then explore how fast the time-averaged probability distribution converges to this limit. In particular, four upper bounds on the mixing time are given, with tightness determined by our knowledge of the quantum walk. For the limiting distribution itself, we study a matrix that encodes the limiting probabilities over the arcs, called the average mixing matrix. We prove that it is flat, that is, all entries are of constant modulus, if and only if $U$ has simple eigenvalues with flat eigenprojections; this is a useful characterization as flat average mixing matrix guarantees uniform limiting distribution over the vertices, regardless of the initial state. Finally, we extend some results on the average mixing matrix in continuous quantum walks to discrete quantum walks. The majority of this chapter comes from Godsil and Zhan [36].

## 3.1 Density Matrices

Let $X$ be a digraph with $m$ arcs. A discrete quantum walk on $X$ is determined by some unitary transition matrix $U$ acting on $\mathbb{C}^m$. Given initial state $x_0$, at step $k$, the system is in state

$$x_k := U^k x_0.$$

If we perform a measurement in the standard basis, then the quantum walker is found on arc $a$ with probability

$$P_{x_0,a}(k) := \left|\langle e_a, U^k x_0\rangle\right|^2.$$

We may express the right hand side using the trace inner product, that is,

$$\left|\langle e_a, U^k x_0\rangle\right|^2 = e_a^T (U^k)^* x_0 x_0^* U^k e_a = \langle (U^k)^* x_0 x_0^* U^k, e_a e_a^T\rangle.$$

Note that both $(U^k)^* x_0 x_0^* U^k$ and $e_a e_a^T$ are positive semidefinite matrices with trace one. This motivates us to describe quantum walks in a different way, using density matrices.

A *density matrix* is a positive semidefinite matrix $\rho$ with $\operatorname{tr}(\rho) = 1$. All $m \times m$ density matrices form a convex set, with extreme points being the rank one projections, that is, $\rho = xx^*$ for some unit vector $x \in \mathbb{C}^m$. Thus, there is a one-to-one correspondence between the extreme points and the quantum states we have seen; these states are called *pure states*. The remaining density matrices represent probabilistic ensembles of pure states, also called *mixed states*. For example, if one is uncertain about the system state in $\mathbb{C}^2$, but knows that it is $e_1$ with probability 50%, and $e_2$ with probability 50%, then the density matrix is

$$\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2} e_1 e_1^T + \frac{1}{2} e_2 e_2^T.$$

However, we also have

$$\frac{1}{2}\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ \frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}}\end{pmatrix} + \frac{1}{2}\begin{pmatrix}\frac{1}{\sqrt{2}}\\ -\frac{1}{\sqrt{2}}\end{pmatrix}\begin{pmatrix}\frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}}\end{pmatrix},$$

so a density matrix does not necessarily determine the probabilistic ensemble of pure states. For more discussion on pure states and mixed states, see [12, 44, 54].

Now let's revisit the quantum walk on $X$. Suppose we start with a pure state, say $\rho_0 = x_0 x_0^*$. At step $k$, the system is in state

$$\rho_k := U^k \rho_0 (U^k)^*.$$

If we perform a measurement in the standard basis, then the system collapses to state $e_a e_a^T$ with probability

$$P_{\rho_0,a}(k) = \langle \rho_k, e_a e_a^T \rangle,$$

that is, the inner product of the pre-measurement state and post-measurement state.

As a special case, when $\rho_0 = e_b e_b^T$ for some arc $e_b$, the probability $P_{\rho_0,a}(k)$ is simply the $ab$-entry of the following Schur product:

$$U^k \circ \overline{U^k};$$

we will refer to this matrix as the *mixing matrix* at step $k$.

What about the probability that the walker is on a vertex $u$? This is defined to be the sum of $P_{\rho_0,a}(k)$ over all outgoing arcs $a$ of $u$. More generally, for any subset $S$ of the arcs of $X$, the probability that the walker is on $S$ at time $k$ is

$$P_{\rho_0,S}(k) := \sum_{a\in S} P_{\rho_0,a}(k).$$

If $\rho_S$ is the uniform mixed state over $S$, that is,

$$\rho_S := \frac{1}{|S|}\sum_{a\in S} e_a e_a^T,$$

then

$$P_{x_0,S}(k) = |S|\langle \rho_k, \rho_S\rangle. \tag{3.1.1}$$

This will be the main formula we use when dealing with the limiting distribution.

## 3.2 Average States and Average Probabilities

A well-known fact about classical random walks is that the probability distribution converges to a stationary distribution, under only mild conditions. Thus it is natural to ask whether the state or the probability distribution converges in a quantum walk. Unfortunately, since $U$ preserves the difference between states at two consecutive steps, neither $\rho_k$ nor $P_{\rho_0,S}(k)$ converges, unless $\rho_1 = \rho_0$. (For a detailed explanation, see Aharonov et al [2].)

Nonetheless, the Cesàro sums of both $\{\rho_k\}$ and $\{P_{\rho_0,S}(k)\}$ exist. The first Cesàro sum,

$$\lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} \rho_k,$$

is called the *average state*; it was proposed by von Neumann as a first step towards thermalization [61]. We will give a formula for the average state using the spectral idempotents of $U$, and apply it to find the second Cesàro sum, the *average probability*:

$$\lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k).$$

**3.2.1 Lemma.** *Let $U$ be a unitary matrix with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*We have*

$$\frac{1}{K}(U^k)\rho_0(U^k)^* = \sum_r F_r\rho_0F_r + \frac{1}{K}\sum_{r\neq s}\left(\frac{1-e^{iK(\theta_r-\theta_s)}}{1-e^{i(\theta_r-\theta_s)}}\right) F_r\rho_0F_s.$$

*Proof.* By the spectral decomposition of $U^k$,

$$\begin{aligned}(U^k)\rho_0(U^k)^* &= \sum_{r,s} e^{ik(\theta_r-\theta_s)}F_r\rho_0F_s \\ &= \sum_r F_r\rho_0F_r + \sum_{r\neq s} e^{ik(\theta_r-\theta_s)}F_r\rho_0F_s.\end{aligned}$$

Hence

$$\begin{aligned}\frac{1}{K}\sum_{k=0}^{K-1} U^k \rho_0 (U^k)^* &= \sum_r F_r\rho_0 F_r + \frac{1}{K}\sum_{r\neq s}\left(\sum_{k=0}^{K-1} e^{ik(\theta_r-\theta_s)}\right) F_r\rho_0 F_s \\ &= \sum_r F_r\rho_0 F_r + \frac{1}{K}\sum_{r\neq s}\left(\frac{1-e^{iK(\theta_r-\theta_s)}}{1-e^{i(\theta_r-\theta_s)}}\right) F_r\rho_0 F_s. \qquad \square\end{aligned}$$

**3.2.2 Theorem.** *Let $U$ be a unitary matrix with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*Given initial state $\rho_0$, the average state of the quantum walk with $U$ as the transition matrix is*

$$\lim_{K\to\infty} \frac{1}{K}\sum_{k=0}^{K-1} \rho_k = \sum_r F_r \rho_0 F_r.$$

*Proof.* By Lemma 3.2.1, it suffices to prove that each entry in the residual

$$\frac{1}{K}\sum_{k=0}^{K-1} U^k\rho_0(U^k)^* - \sum_r F_r\rho_0 F_r$$

is bounded by some constant independent of $K$. Indeed, for any $K$ and any $r \neq s$,

$$\left|\frac{1-e^{iK(\theta_r-\theta_s)}}{1-e^{i(\theta_r-\theta_s)}}\right| \leq \frac{2}{|1-e^{i(\theta_r-\theta_s)}|},$$

which only depends on $r$ and $s$. $\square$

The map

$$\rho_0 \mapsto \sum_r F_r\rho_0 F_r$$

is knowns as the conditional expectation onto the commutant of $U$. We give another interpretation of this map from a channel viewpoint. For backgound on quantum channels, see [12, 44, 54]. Since the eigenprojections satisfy

$$\sum_r F_r^* F_r = I,$$

the mapping on density matrices given by

$$\rho_0 \mapsto \sum_r F_r \rho_0 F_r^*$$

is a quantum channel. Therefore, the time-averaged state is effectively the image of the initial state passing through this channel.

The formula for the average probability now follows from Equation (3.1.1).

**3.2.3 Theorem.** *Let $X$ be a digraph. Let $U$ be a transition matrix of a quantum walk on $X$, with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*Given initial state $\rho_0$ and a subset $S$ of arcs, the average probability of the quantum walker being on $S$ is*

$$\lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k) = |S| \sum_r \langle F_r \rho_0 F_r, \rho_S \rangle.$$ □

Two questions about the average probability are of our interest: how fast does the partial sum

$$\frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k)$$

converge, and when is the average probability distribution uniform? We will investigate these in the next two sections, respectively.

## 3.3 Mixing Times

Given $\epsilon > 0$, the *mixing time* $M_{\rho_0,S}(\epsilon)$ with respect to initial state $\rho_0$ and target arcs $S$ is the smallest $L$ such that for all $K > L$,

$$\left| \frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k) - |S| \sum_r \langle F_r \rho_0 F_r, \rho_S \rangle \right| \le \epsilon.$$

There are several variants of this definition. For instance, we may consider the mixing time conditioned on the initial state being any standard basis vector:

$$M_S(\epsilon) := \sup\{M_{\rho_0,S}(\epsilon) : \rho_0 = e_a e_a^T \text{ for some arc } a\},$$

For a more global purpose, we could look at the smallest $L$ such that for all $K > L$, the average probability distribution over vertices is $\epsilon$-close to the limiting distribution over vertices. In [2], Aharonov et al studied the mixing time of the last type, and obtained an upper bound for a general graph. They further showed that the mixing time of a quantum walk on an $n$-cycle with the Hadamard coin is bounded above by $O(n \log n)$, giving a quadratic speedup over the classical random walk. We now extend some of their results on mixing times of the form $M_{\rho_0,S}(\epsilon)$.

**3.3.1 Theorem.** *Let $X$ be a digraph. Let $U$ be a transition matrix of a quantum walk on $X$, with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*Given initial state $\rho_0$ and a subset $S$ of arcs, the mixing time $M_{\rho_0,S}(\epsilon)$ satisfies*

$$M_{\rho_0,S}(\epsilon) \leq \frac{2|S|}{\epsilon} \sum_{r \neq s} \frac{|\langle F_r \rho_0 F_s, \rho_S \rangle|}{|e^{i\theta_r} - e^{i\theta_s}|} \tag{3.3.1}$$

$$\leq \frac{2}{\epsilon} \sum_{r \neq s} \sum_{a \in S} \frac{\sqrt{(F_r)_{aa}(F_s)_{aa}}}{|e^{i\theta_r} - e^{i\theta_s}|} \tag{3.3.2}$$

$$\leq \frac{2|S|}{\epsilon} \sum_{r \neq s} \frac{1}{|e^{i\theta_r} - e^{i\theta_s}|} \tag{3.3.3}$$

$$\leq \frac{2\ell|S|}{\epsilon\Delta}, \tag{3.3.4}$$

*where $\ell$ is the number of pairs of distinct eigenvalues, and*

$$\Delta := \min\{\left|e^{i\theta_r} - e^{i\theta_s}\right| : r \neq s\}.$$

*Proof.* From Lemma 3.2.1 we see that

$$\begin{aligned}\left|\frac{1}{K} P_{\rho_0,S}(k) - |S| \sum_r \langle F_r \rho_0 F_r, \rho_S \rangle \right| &= \frac{|S|}{K} \left| \sum_{r \neq s} \frac{1 - e^{iK(\theta_r - \theta_s)}}{1 - e^{i(\theta_r - \theta_s)}} \langle F_r \rho_0 F_s, \rho_S \rangle \right| \\ &\leq \frac{|S|}{K} \sum_{r \neq s} \left| \frac{1 - e^{iK(\theta_r - \theta_s)}}{1 - e^{i(\theta_r - \theta_s)}} \right| |\langle F_r \rho_0 F_s, \rho_S \rangle| \\ &\leq \frac{2|S|}{K} \sum_{r \neq s} \frac{|\langle F_r \rho_0 F_s, \rho_S \rangle|}{|e^{i\theta_r} - e^{i\theta_s}|} \end{aligned} \tag{3.3.5}$$

$$= \frac{2|S|}{K} \sum_{r \neq s} \frac{|\langle \rho_0, F_r \rho_S F_r \rangle|}{|e^{i\theta_r} - e^{i\theta_s}|}$$

$$\leq \frac{2|S|}{K} \sum_{r \neq s} \frac{\|F_r \rho_S F_s\|}{|e^{i\theta_r} - e^{i\theta_s}|}$$

$$\leq \frac{2}{K} \sum_{r \neq s} \sum_{a \in S} \frac{\sqrt{(F_r)_{aa}(F_s)_{aa}}}{|e^{i\theta_r} - e^{i\theta_s}|} \tag{3.3.6}$$

$$\leq \frac{2|S|}{K} \sum_{r \neq s} \frac{1}{|e^{i\theta_r} - e^{i\theta_s}|} \tag{3.3.7}$$

$$\leq \frac{2\ell|S|}{K\Delta}. \tag{3.3.8}$$

Thus, for all $K$ such that

$$K > \frac{2|S|}{\epsilon} \sum_{r \neq s} \frac{|\langle F_r \rho_0 F_s, \rho_S \rangle|}{|e^{i\theta_r} - e^{i\theta_s}|},$$

the right hand side of Inequality (3.3.5) is no more than $\epsilon$. Similarly, the other three bounds follow from Inequalities (3.3.6), (3.3.7) and (3.3.8). □

The last bound in Theorem 3.3.1 is equivalent to Lemma 4.3 in Aharonov et al [2]. The other three bounds are stronger, but require more knowledge of the quantum walk besides the eigenvalues of $U$.

Below we present some data on the four upper bounds for two models on the circulant graph $X = X(\mathbb{Z}_n, \{1, -1, 2, -2\})$. Choose an initial state that concentrate on vertex 0, that is,

$$\rho_0 = \frac{1}{4} E_{00} \otimes J.$$

Let $S_v$ denote the set of outgoing arcs of vertex $v$. For each upper bound $\beta_{\rho_0,S}$ in (3.3.1) , 3.3.2), (3.3.3), and (3.3.4), we compute

$$\frac{\epsilon}{2} \sum_{v \in \mathbb{Z}_n} \beta_{\rho_0, S_v},$$

and store them in Table 3.1.

The models we consider are the arc-reversal Grover walk, which we introduced in Chapter 2, and the shunt-decomposition Grover walk, which we will introduce in Chapter 4. Let $U_{ar}$ be the transition matrix of the arc-reversal Grover walk on $X$, and $U_{sd}$ the transition matrix of the shunt-decomposition Grover walk on $X$. One can verify that if the spectral decomposition of $U_{ar}$ is

$$U_{ar} = \sum_r \alpha_r F_r,$$

then the spectral decomposition of $U_{sd}$ is

$$U_{sd} = \sum_r -\alpha_r F'_r,$$

where for any $r$, the eigenprojections $F_r$ and $F'_r$ have the same diagonal. Thus, the upper bounds 3.3.2), (3.3.3) and (3.3.4) are identical for both models. However, the last two columns in Table 3.1 indicates a difference between these two models—the shunt-decomposition Grover walk may have a lower mixing time than the arc-reversal Grover walk.

## 3.4 Average Mixing Matrix

Let $X$ be a digraph. Let $U$ be a transition matrix of a quantum walk on $X$, with spectral decomposition

$$U = \sum_r e^{i\theta_r} F_r.$$

In this section, we pay special attention to the average probability of the quantum walk from one arc $a$ to another arc $b$, that is,

$$\sum_r \langle F_r e_a e_a^T F_r, e_b e_b^T \rangle.$$

Note that this is precisely the $ab$-entry of $\sum_r F_r \circ \overline{F_r}$. Following Godsil's notion for continuous quantum walks [28], we let

$$\widehat{M} := \sum_r F_r \circ \overline{F_r},$$

and call $\widehat{M}$ the *average mixing matrix*. Theorem 3.2.3 implies that

$$\widehat{M} = \lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} U^k \circ \overline{U^k}.$$

| $n$ | (3.3.4) ar/sd | (3.3.3) ar/sd | (3.3.2) ar/sd | (3.3.1) ar | (3.3.1) sd |
|---|---|---|---|---|---|
| 6 | 1390.93 | 598.05 | 85.19 | 1.69 | 0.91 |
| 7 | 4620.05 | 1516.4 | 148.57 | 2.61 | 1.91 |
| 8 | 17771.88 | 3408.35 | 240.94 | 4.29 | 2.36 |
| 9 | 24838.95 | 3991.5 | 287.33 | 4.82 | 1.73 |
| 10 | 14285.23 | 3687.22 | 269.22 | 4.49 | 2.12 |
| 11 | 95452.33 | 9092.93 | 508.32 | 6.7 | 2.97 |
| 12 | 23505.04 | 4678.44 | 348.8 | 4.25 | 2.45 |
| 13 | 79048.14 | 13277.27 | 640.52 | 8.06 | 3.09 |
| 14 | 148284.47 | 19895.81 | 803.94 | 10.1 | 3.97 |
| 15 | 225507.28 | 16355.5 | 764.76 | 9.33 | 2.46 |
| 16 | 371901.16 | 34910.54 | 1211.24 | 13.57 | 4.96 |
| 17 | 2591443.27 | 65759.41 | 2127.89 | 24.26 | 5.54 |
| 18 | 330012.11 | 36141.49 | 1284.51 | 13.45 | 4.39 |
| 19 | 4854951.51 | 94822.86 | 2743.75 | 33.37 | 6.24 |
| 20 | 518641.81 | 51235.99 | 1562.68 | 15.33 | 5.37 |
| 21 | 848915.39 | 70921.92 | 1994.95 | 17.94 | 5.04 |
| 22 | 4443833.25 | 129338.06 | 3143.36 | 28.53 | 7.97 |
| 23 | 1651611.78 | 101994.04 | 2577.25 | 21.63 | 6.41 |
| 24 | 887647.03 | 76568.55 | 2185.39 | 18.05 | 6.69 |
| 25 | 1715366.87 | 103250.55 | 2603.42 | 20.88 | 5.9 |

Table 3.1: Upper bounds for the mixing time on $X(\mathbb{Z}_n, \{1, 2, -1, -2\})$

In [28], Godsil established several properties of the continuous average mixing. We extend some of his results to discrete quantum walks.

The first observation is that $\widehat{M}$ is doubly-stochastic. Moreover, since each $F_r$ is Hermitian, $\widehat{M}$ is symmetric although $U^k \circ \overline{U^k}$ is not. Thus we can view either the $a$-th row or the $a$-th column of $\widehat{M}$ as the average probability distribution given initial state $e_a e_a^T$.

For a continuous quantum walk, the average mixing matrix is proved to be positive semidefinite with eigenvalues no greater than one [28]. We show that the same statement holds for the discrete average mixing matrix.

**3.4.1 Lemma.** *The average mixing matrix $\widehat{M}$ of a quantum walk is positive semidefinite, and its eigenvalues lie in* $[0, 1]$.

*Proof.* Since $F_r$ is positive semidefinite, its complex conjugate $\overline{F_r}$ is positive semidefinite as well. Hence $F_r \otimes \overline{F_r}$ is positive semidefinite. As a principal submatrix of $F_r \otimes \overline{F_r}$, the Schur product $F_r \circ \overline{F_s}$ must also be positive semidefinite. Therefore, the eigenvalues of $\widehat{M}$ are non-negative. It follows from

$$I = I \circ I = \left(\sum_r F_r\right) \circ \left(\sum_s \overline{F_s}\right) = \widehat{M} + \sum_{r \neq s} F_r \circ \overline{F_s}$$

and the positive-semidefiniteness of $F_r \circ \overline{F_s}$ that the eigenvalues of $\widehat{M}$ are at most 1. On the other hand, since $\widehat{M}$ is doubly stochastic, **1** is an eigenvector for $\widehat{M}$ with eigenvalue 1. □

To measure the flatness of $\widehat{M}e_a$, we define its *entropy* to be the negative expectation of the logarithm of its entries, that is,

$$-\sum_b \widehat{M}_{ab} \log(\widehat{M}_{ab}).$$

This quantity reaches maximum if and only if the probability distribution $\widehat{M}e_a$ is uniform. Likewise, the *total entropy* of $\widehat{M}$ is

$$-\sum_{a,b} \widehat{M}_{ab} \log(\widehat{M}_{ab});$$

it is maximized when the entire average mixing matrix is flat. In [10], Bai, Rossi, Cui, and Hancock proposed a graph signature based on the total entropy of continuous quantum walks. According to their experimental results, this entropic measure provides significant information on the properties of graphs.

A quantum walk with flat $\widehat{M}$ is said to admit *uniform average mixing*. According to the definition of $\widehat{M}$, uniform average mixing means that, in the limit, the walker has equal chance of being on any arc, no matter which arc she started with. In fact, as we will see later, something stronger is true when $\widehat{M}$ is flat—the average probability distribution is uniform over all the arcs, regardless of the initial state.

While $\widehat{M}$ contains complete information on the average probabilities from arcs to arcs, one may be interested in average probabilities on the vertices as well. We say a quantum walk admits *uniform average vertex mixing* if the walker has equal chance of being on any vertex in the limit, regardless of the initial state.

Our next goal is to establish necessary and sufficient conditions for uniform average mixing to occur.

**3.4.2 Lemma.** *Let $U$ be an $m \times m$ unitary matrix with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*If $\ell_r$ is the multiplicity of the $r$-th eigenvalue of $U$, then*

$$\operatorname{tr}(\widehat{M}) \geq \frac{1}{m} \sum_r \ell_r^2.$$

*Further, equality holds if and only if each idempotent $F_r$ has constant diagonal.*

*Proof.* Since $F_r$ is positive semidefinite, its diagonal entries are non-negative and

$$\operatorname{tr}(F_r) = \ell_r.$$

By Cauchy-Schwarz,

$$\operatorname{tr}(F_r \circ \overline{F_r}) \geq \frac{1}{m} \operatorname{tr}(F_r)^2 = \frac{1}{m} \ell_r^2.$$

Hence

$$\operatorname{tr}(\widehat{M}) \geq \frac{1}{m} \sum_r \ell_r^2.$$

Equality holds if and only if each $F_r$ has constant diagonal $\ell_r/m$. □

**3.4.3 Corollary.** *Let $U$ be a unitary matrix, and $\widehat{M}$ the associated average mixing matrix.Then $\operatorname{tr}(\widehat{M}) \geq 1$, with equality held if and only if $U$ has simple eigenvalues with flat eigenprojections.*

*Proof.* Note that

$$\sum_r \ell_r = m.$$

By Lemma 3.4.2 and Cauchy-Schwarz,

$$\operatorname{tr}(\widehat{M}) \geq \frac{1}{m} \sum_r \ell_r^2 \geq 1.$$

Equality holds if and only if for all $r$, the idempotent $F_r$ is a rank-one projection with constant diagonal, that is, each eigenvalue is simple with flat eigenprojections. □

With all tools established, we are ready to characterize uniform average mixing in discrete quantum walks.

**3.4.4 Theorem.** *Let $U$ be a transition matrix of a quantum walk, and $\widehat{M}$ the associated average mixing matrix. The following statements are equivalent.*

*(i) The quantum walk admits uniform average mixing.*

*(ii)* $\operatorname{tr}(\widehat{M}) = 1$.

*(iii) $U$ has simple eigenvalues with flat eigenprojections.*

*Proof.* If uniform average mixing occurs, then all entries of $\widehat{M}$ are equal to $1/m$, so $\operatorname{tr}(\widehat{M}) = 1$. Hence (i) implies (ii). It follows from Corollary 3.4.3 that (ii) implies (iii). Now suppose (iii) holds. Then the spectral decomposition of $U$ is

$$U = \sum_{r=1}^{m} e^{i\theta_r} F_r,$$

where for each $r$, all entries in $F_r$ have the same absolute value. Hence

$$\widehat{M}_{ab} = \sum_{r=1}^{m} (F_r \circ \overline{F_r})_{ab} = \sum_{r=1}^{m} |(F_r)_{ab}|^2,$$

which does not depend on $a$ and $b$. Therefore (iii) implies (i). □

What about average probabilities on vertices, or subsets of arcs? The following result shows that if $\widehat{M}$ is flat, then the average probability that the walker is on some subset $S$ of arcs depends only on the size $|S|$. In particular, uniform average mixing implies uniform average vertex mixing.

**3.4.5 Theorem.** *Let $X$ be a digraph. If a quantum walk on $X$ admits uniform average mixing, then for any initial state $\rho_0$ and any arc set $S$,*

$$\lim_{K\to\infty} \frac{1}{K} \sum_{k=0}^{K-1} P_{\rho_0,S}(k) = \frac{|S|}{nd}.$$

*Proof.* Suppose uniform average mixing occurs. By Theorem 3.4.4, we can write the spectral decomposition of $U$ as

$$U = \sum_{r=1}^{m} e^{i\theta_r} F_r,$$

where each $F_r$ is a rank-one flat matrix. By Theorem 3.2.3,

$$\begin{aligned}\lim_{K\to\infty}\frac{1}{K}\sum_{k=0}^{K-1}P_{\rho_0,S}(k) &= |S|\sum_{r=1}^{m}\langle F_r\rho_0F_r,\rho_S\rangle\\ &= |S|\sum_{r=1}^{m}\langle \rho_0, F_r\rho_S F_r\rangle\\ &= \frac{|S|}{nd}\sum_{r=1}^{m}\langle\rho_0,F_r\rangle\\ &= \frac{|S|}{nd}\langle\rho_0,I\rangle\\ &= \frac{|S|}{nd}\end{aligned}$$

□

The converse of Theorem 3.4.5 is not true. In fact, neither simple eigenvalues nor flat eigenvectors are necessary for uniform average vertex mixing. Later in Chapter 4, we will construct an infinite family of quantum walks that admit uniform average vertex mixing, where the transition matrices do not have simple eigenvalues; these are quantum walks on circulant digraphs.

To end this section, we prove some algebraic properties of $\widehat{M}$. They rely on the well-known fact that a commutative semisimple matrix algebra with identity has a basis of orthogonal idempotents. In continuous quantum walks, similar results turn out to be quite useful in determining uniform mixing; see for example [33]. We hope the analogy in discrete quantum walks will be of use too.

**3.4.6 Theorem.** *Let $U$ be the transition matrix of a quantum walk, and $\widehat{M}$ the associated average mixing matrix. If the entries of $U$ are algebraic over $\mathbb{Q}$, then the entries of $\widehat{M}$ are algebraic over $\mathbb{Q}$.*

*Proof.* Suppose $U$ has algebraic entries. Then its eigenvalues are all algebraic. Let $\mathbb{F}$ be the smallest field containing the eigenvalues of $U$. Let $\mathcal{B}$ be the matrix algebra generated by $U$ over $\mathbb{F}$. To show that $\mathcal{B}$ is semisimple, pick $N \in \mathcal{B}$ with $N^2 = 0$. Since $U$ is unitary, the algebra $\mathcal{B}$ is closed under conjugate transpose and contains the identity. It follows from $(N^*)^2 = 0$ that

$$0 = \operatorname{tr}((N^*)^2 N^2)$$

$$= \operatorname{tr}(N^*NN^*N)$$
$$= \operatorname{tr}((N^*N)^*(N^*N)).$$

Thus $N^*N = 0$. Applying the trace again to $N^*N$, we see that $N = 0$. Therefore, the spectral idempotents $F_r$ of $U$ are polynomials in $U$ with algebraic coefficients. Hence the entries in

$$\widehat{M} = \sum_r F_r \circ \overline{F_r}$$

are algebraic over $\mathbb{Q}$. □

In continuous quantum walks, the entries of the average mixing matrix are all rational [28]. We show that the discrete average mixing matrix enjoys the same property, given that all entries of $U$ are rational.

**3.4.7 Theorem.** *Let $U$ be the transition matrix of a quantum walk, and $\widehat{M}$ the associated average mixing matrix. If the entries of $U$ are rational, then the entries of $\widehat{M}$ are rational.*

*Proof.* Let the spectral decomposition of $U$ be

$$U = \sum_r \alpha_r F_r.$$

Let $\mathbb{F}$ be the smallest field containing the eigenvalues of $U$. Let $\sigma$ be an automorphism of $\mathbb{F}$. Since $U$ is rational, we have

$$U = U^\sigma = \sum_r \alpha_r^\sigma F_r^\sigma.$$

Moreover, since $\alpha_r^\sigma$ is also an eigenvalue of $U$, the set of idempotents $\{F_r\}$ is closed under field automorphisms. Thus

$$\widehat{M} = \sum_r F_r \circ F_r^T$$

is fixed by all automorphisms of $\mathbb{F}$ and must be rational. □

# Chapter 4

# Specifying Directions

In Chapter 2, our quantum walker jumps from an arc to its inverse after each coin flip. However, this is not the only way she could move. If the graph is a cycle, each arc points either clockwise or counterclockwise, so she may jump between consecutive arcs with the same direction. Similarly, if the graph is a grid on the torus, she may move one step up, down, left, or right according to where the current arc points.

In this chapter, we study quantum walks on digraphs where such "directions" can be specified. We show that specifying $d$ directions on a digraph $X$ is equivalent to expressing its adjacency matrix as a sum of $d$ permutation matrices, called shunts. Consequently, $X$ must be $d$-regular, that is, every vertex has $d$ out-neighbors and $d$ in-neighbors.

While the transition matrix $U$ still lies in a dihedral group, its spectrum is in general harder to obtain, so we focus on the case where all the shunts commute, that is, when $X$ is a Cayley digraph over an abelian group $\Gamma$. Given that every vertex receives the same coin, the spectral decomposition of $U$ is determined by the coin and the characters of $\Gamma$; this was originally observed by Aharonov et al [2]. We apply their results to shunt-decomposition Grover walks, and obtain explicit formulas for the eigenvalues and eigenvectors.

As pointed out in [2], a shunt-decomposition walk admits uniform average vertex mixing if $U$ has distinct eigenvalues. With Grover coins, however, $U$ will always have $-1$ as a non-simple eigenvalue unless $d = 2$. Therefore, previous studies on uniform average vertex mixing concentrated on cycles with more complicated coins. We show that for a shunt-decomposition Grover walk, the simple-eigenvalue condition is unnecessary, thus opening up possibilities for more examples with higher degrees. Using tools from algebraic number theory, we prove that for any prime $p$, a 3-regular circulant digraph over $\mathbb{Z}_p$ admits uniform average vertex mixing if and only if its connection set has trivial stabilizer in $\mathrm{Aut}(\mathbb{Z}_p)$. This provides the first infinite family of digraphs, other than cycles, that admit uniform average mixing. We believe a similar characterization works when the degree is greater than 3.

Finally, we give an overview of a different approach to shunt-decomposition walks on infinite graphs, due to Ambainis et al [4]. This was the first paper on shunt-decomposition models where exact analysis was carried out.

## 4.1 Shunt-Decomposition Walks

Assume $X$ is a $d$-out-regular digraph, so that we can assign $d$ "directions" to each vertex. In this section, we discuss what other conditions $X$ must satisfy, to allow a quantum walk that respects these directions. This type of quantum walk was first introduced by Aharonov et al [2].

Note that any assignment of $d$ directions partitions the arcs into $d$ groups, each of which induces a digraph with out-valency one. Let $A_1, A_2, \ldots, A_d$ be the adjacency matrices of these digraphs. If $S$ is the matrix sending arc $(u, v)$ to arc $(v, w)$ in the same group, then it can be written as

$$S = \begin{pmatrix} A_1^{-1} & & & \\ & A_2^{-1} & & \\ & & \ddots & \\ & & & A_d^{-1} \end{pmatrix}.$$

We would like to modify an arc-reversal walk in the following way: keep the coin matrix, and replace the arc-reversal operator $R$ with the directional shift operator $S$. Note that the transition matrix is unitary if and only if $S$ is unitary, and $S$ is unitary if and only if each $A_j$ defines a permutation on $V(X)$.

A permutation on $V(X)$ that maps each vertex to a neighbor is called a *shunt*. Given $d$ shunts $P_1, P_2, \ldots, P_d$, the decomposition

$$A(X) = P_1 + \cdots + P_d,$$

is called a *shunt-decomposition* of $X$. Any digraph that admits a shunt-decomposition must be both $d$-in-regular and $d$-out-regular, or *$d$-regular* for short. We show that the converse is also true.

**4.1.1 Lemma.** *Let $X$ be a $d$-regular digraph. Then $X$ admits a shunt-decomposition.*

*Proof.* Let $A$ be the adjacency matrix of $X$. Define

$$B := \begin{pmatrix} 0 & A \\ A^T & 0 \end{pmatrix}.$$

Then $B$ is the adjacency matrix of a $d$-regular bipartite graph. It is a well-known fact that every regular bipartite graph has a 1-factorization, whence

$$B = \begin{pmatrix} 0 & P_1 \\ P_1^T & 0 \end{pmatrix} + \cdots + \begin{pmatrix} 0 & P_d \\ P_d^T & 0 \end{pmatrix},$$

where $P_1, P_2, \ldots, P_d$ are permutation matrices. Therefore,

$$A(X) = P_1 + \cdots + P_d.$$ □

In the rest of this chapter, assume $X$ is a $d$-regular digraph. Let $C$ be a $d \times d$ unitary coin. As with the arc-reversal $C$-walk (see Section 2.2), for each vertex $u$, we need to specify a linear order on the neighbors of $u$:

$$f_u : \{1, 2, \cdots, \deg(u)\} \to \{v : u \sim v\},$$

in order to construct the coin matrix. One way to do this is to choose the linear order $f_u$ according to a shunt-decomposition of $X$:

$$A(X) = P_1 + \cdots + P_d;$$

that is, for $j = 1, 2, \cdots, d$, set $f_u(j) = e_v$ where $v$ is the unique vertex such that

$$P_j^{-1} e_u = e_v.$$

Given linear orders

$$\{f_u : u \in V(X)\},$$

the coin $C$ sends $(u, f_u(j))$ to a superposition of all outgoing arcs of $u$, in which the amplitudes come from the $j$-th column of $C$:

$$Ce_j = \sum_{k=1}^{d} (e_k^T C e_j) e_k.$$

Now let

$$A(X) = P_1 + \cdots + P_d$$

be a shunt-decomposition of $X$, and let

$$S = \begin{pmatrix} P_1^{-1} & & & \\ & P_2^{-1} & & \\ & & \ddots & \\ & & & P_d^{-1} \end{pmatrix}.$$

The ordering of the rows and columns of $S$ defines a set of linear orders $\{f_u : u \in V(X)\}$. Choose a $d \times d$ unitary coin $C$, and assign it to each vertex $u$ according to $f_u$. Then the coin matrix can be written as $C \otimes I$. The unitary matrix

$$U = S(C \otimes I)$$

is the transition matrix of a *shunt-decomposition $C$-walk* on $X$.

Note that $S$ has finite order $n$. In general, $S$ and $C \otimes I$ do not commute, and the spectral decomposition of $U$ could be very hard to derive. However, if $P_1, P_2, \ldots, P_d$ have a common eigenvector $\chi$, then we can use $\chi$ to construct an eigenvector for $U$. This observation is due to Aharonov et al [2].

**4.1.2 Lemma.** *Let $X$ be a digraph with shunt-decomposition*

$$A(X) = P_1 + \cdots + P_d.$$

*Let $U$ be the transition matrix of a shunt-decomposition $C$-walk on $X$. Let $\chi$ be a common eigenvector for the shunts $P_1, P_2, \ldots, P_d$ with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_d$, respectively. Then $y \otimes \chi$ is an eigenvector for $U$ with eigenvalue $\alpha$ if and only if $y$ is an eigenvector for*

$$\begin{pmatrix} \lambda_1^{-1} & & & \\ & \lambda_2^{-1} & & \\ & & \ddots & \\ & & & \lambda_d^{-1} \end{pmatrix} C$$

*with eigenvalue $\alpha$.*

*Proof.* We have

$$U(y \otimes \chi) = \begin{pmatrix} P_1^{-1} & & & \\ & P_2^{-1} & & \\ & & \ddots & \\ & & & P_d^{-1} \end{pmatrix} (Cy \otimes \chi)$$

$$= \sum_{j=1}^{d} (E_{jj}Cy) \otimes (P_j^{-1}\chi)$$
$$= \left( \left( \sum_{j=1}^{d} \lambda_j^{-1} E_{jj} \right) Cy \right) \otimes \chi$$
$$= \left( \begin{pmatrix} \lambda_1^{-1} & & & \\ & \lambda_2^{-1} & & \\ & & \ddots & \\ & & & \lambda_d^{-1} \end{pmatrix} Cy \right) \otimes \chi.$$

Thus

$$U(y \otimes \chi) = \alpha(y \otimes \chi)$$

if and only if

$$\begin{pmatrix} \lambda_1^{-1} & & & \\ & \lambda_2^{-1} & & \\ & & \ddots & \\ & & & \lambda_d^{-1} \end{pmatrix} Cy = \alpha y.$$ □

## 4.2 Commuting Shunts and Grover coins

In this section, we study the spectrum of a shunt-decomposition walk where all the shunts commute. A complete characterization follows from Lemma 4.1.2. We then look into the case where each vertex receives the Grover coin, and obtain more explicit formulas for the eigenvalues and eigenvectors of $U$.

Suppose $X$ has shunt-decomposition

$$A(X) = P_1 + \cdots + P_d,$$

where $P_j P_k = P_k P_j$ for all $j$ and $k$. Then $P_1, P_2, \ldots, P_d$ generate an abelian group $\Gamma$, which acts regularly on the vertices of $X$. Thus, $X$ is isomorphic to a Cayley digraph over $\Gamma$ with connection set $\{P_1, P_2, \ldots, P_d\}$. Since the characters of $\Gamma$ are eigenvectors for the regular representation of $\Gamma$, and distinct characters are orthogonal, by Lemma 4.1.2, they give rise to a basis of eigenvectors for $U$.

From now on, let $\Gamma$ be a finite abelian group, and let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$, denoted

$$X(\Gamma, \{g_1, g_2, \ldots, g_d\}).$$

Since $\Gamma$ is abelian, the images of the connection set under the regular representation of $\Gamma$ are the shunts $P_1, P_2, \ldots, P_d$ in a shunt-decomposition of $X$. If $\chi$ is an character of $\Gamma$, then

$$P_j \chi = \chi(g_j)\chi.$$

Define

$$\Lambda_\chi := \begin{pmatrix} \chi(g_1^{-1}) & & & \\ & \chi(g_2^{-1}) & & \\ & & \ddots & \\ & & & \chi(g_d^{-1}) \end{pmatrix}.$$

The following result, as a consequence of Lemma 4.1.2, is again due to Aharonov et al [2].

**4.2.1 Theorem.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition $C$-walk on $X$. The eigenvalues of $U$ consists of eigenvalues of $\Lambda_\chi C$, where $\chi$ ranges over all characters of $\Gamma$.* □

Note that when $\chi$ is the trivial character, we have $\Lambda_\chi C = C$. Hence the eigenvalues of the coin are always eigenvalues of $U$.

Let $G$ be the $d \times d$ Grover coin. Consider a shunt-decomposition Grover walk. We derive explicit formulas for the eigenvalues of $U$, in terms of the characters. While the following theorem only states what the eigenvalues of $U$ are, the proof also provides a construction for all the eigenvectors.

**4.2.2 Theorem.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. Let $\chi$ be a non-trivial character of $\Gamma$. Each eigenvalue $\alpha$ of $\Lambda_\chi G$ is either*

*(i) a zero of*

$$\frac{1}{\alpha\chi(g_1)+1} + \cdots + \frac{1}{\alpha\chi(g_d)+1} - \frac{d}{2},$$

*with multiplicity 1, or,*

*(ii) $-\chi(g_j^{-1})$, with multiplicity one less than the number of $k$'s such that $\chi(g_k) = \chi(g_j)$.*

*Proof.* Let $y$ be an eigenvector for $\Lambda_\chi G$ with eigenvalue $\alpha$. Since

$$G = \frac{2}{d}J - I,$$

we need to solve

$$\frac{2}{d}Jy = (\alpha\Lambda_\chi^{-1} + I)y,$$

that is,

$$\frac{2}{d}\langle \mathbf{1}, y\rangle \mathbf{1} = \begin{pmatrix} (\alpha\chi(g_1)+1)y_1 \\ \vdots \\ (\alpha\chi(g_d)+1)y_d \end{pmatrix}. \tag{4.2.1}$$

Consider two cases.

(i) Suppose $\langle \mathbf{1}, y\rangle \neq 0$. Then the right hand side in Equation (4.2.1) is a vector with no zero entry. Without loss of generality we may assume $\langle \mathbf{1}, y\rangle = 1$. Thus,

$$\frac{1}{\alpha\chi(g_1)+1} + \cdots + \frac{1}{\alpha\chi(g_d)+1} = \frac{d}{2}, \tag{4.2.2}$$

and each solution $\alpha$ to the above uniquely determines an eigenvector $y$ with $\langle \mathbf{1}, y\rangle = 1$. Therefore the distinct zeros of Equation (4.2.2) are eigenvalues of $\Lambda_\chi G$. Further, if any of them has multiplicity greater than one, then it must have an eigenvector $y$ such that $\langle y, \mathbf{1}\rangle = 0$, which implies one of

$$\alpha(\chi(g_1)+1), \cdots, \alpha(\chi(g_d)+1)$$

is equal to zero, a contradiction.

(ii) Suppose $\langle \mathbf{1}, y\rangle = 0$. Since $y \neq 0$, there must exists some $j$ such that

$$\alpha\chi(g_j) + 1 = 0,$$

that is, $\alpha = -\chi(g_j^{-1})$. Then for any $k$ such that $\chi(g_j) \neq \chi(g_k)$, we have $y_k = 0$. Hence $y$ is orthogonal to $\mathbf{1}$ if and only if

$$\sum_{k:\chi(g_k)=\chi(g_j)} y_j = 0,$$

from which the multiplicity of $\alpha$ follows. □

## 4.3 Uniform Average Vertex Mixing

One topic in the limiting behavior of quantum walks is uniform average vertex mixing. We saw in Section 3.4 that this is guaranteed whenever the average mixing matrix $\widehat{M}$ is flat, or equivalently, when $U$ has simple eigenvalues and flat eigenvectors. However, uniform average vertex mixing does not imply uniform average mixing. The following two results are due to Aharonov et al [2].

**4.3.1 Theorem.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition $C$-walk on $X$, with spectral decomposition*

$$U = \sum_r e^{i\theta_r} F_r.$$

*If $U$ has simple eigenvalues, and for each $r$, $\langle F_r, \rho_S \rangle = 1$ whenever $S$ is is the set of outgoing arcs of a vertex, then $U$ admits uniform average vertex mixing.* □

**4.3.2 Corollary.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition $C$-walk on $X$. If $U$ has simple eigenvalues, then the quantum walk admits uniform average vertex mixing.*

*Proof.* This follows immediately from the structure of eigenvectors for $U$, as described in Lemma 4.1.2. □

Using these results, Aharonov et al [2] showed that on every odd cycle, the shunt-decomposition Hadamard walk admits uniform average mixing. We wish to construct more examples with Grover coins.

Let $X$ be a $d$-regular Cayley digraph over an abelian group $\Gamma$, and let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. The first difficulty we face is that when $d > 2$, the coin $G$ itself contributes $-1$ to the spectrum of $U$ at least twice. Hence the above corollary no longer applies. Fortunately, simple eigenvalues are not necessary for uniform average vertex mixing to occur; a slightly weaker condition also works.

**4.3.3 Theorem.** *Let $\Gamma$ be a finite abelian group. Let $X$ be a Cayley digraph over $\Gamma$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of* *a shunt-decomposition Grover walk on $X$. If the only non-simple eigenvalue of $U$ is $-1$ with multiplicity $d-1$, then $U$ admits uniform average vertex mixing.*

*Proof.* Suppose $X$ has $n$ vertices. Since $-1$ is an eigenvalue of $U$ with multiplicity $d-1$, by Lemma 4.1.2 and Theorem 4.2.2, the eigenprojection of $-1$ must be

$$F_{-1} = \left(I - \frac{1}{d}J\right) \otimes \frac{1}{n}J.$$

Let $u$ be any vertex of $X$, and $S$ the set of outgoing arcs of $X$. Then

$$\begin{aligned} F_{-1}\rho_S F_{-1} &= \frac{1}{d}\left(\left(I - \frac{1}{d}J\right) \otimes \frac{1}{n}J\right)(I \otimes E_{uu})\left(\left(I - \frac{1}{d}J\right) \otimes \frac{1}{n}J\right) \\ &= \frac{1}{n^2 d}\left(I - \frac{1}{d}J\right) \otimes (JE_{uu}J) \\ &= \frac{1}{nd}F_{-1}. \end{aligned}$$

On the other hand, since the remaining eigenvalues are all simple, we have

$$F_r \rho_S F_r = \frac{1}{nd}F_r$$

for all $r \neq -1$. Thus by Theorem 3.2.3,

$$\begin{aligned} \lim_{K\to\infty} \frac{1}{K}\sum_{k=0}^{K-1} P_{\rho_0,S}(k) &= d\sum_{r=1}^{m} \langle F_r\rho_0F_r, \rho_S\rangle \\ &= d\sum_{r} \langle \rho_0, F_r\rho_S F_r\rangle \\ &= \frac{1}{n}\sum_{r} \langle \rho_0, F_r\rangle \\ &= \frac{1}{n}. \end{aligned}$$

□

Combining this with Theorem 4.2.2, we need a Cayley digraph where

$$\chi(g_1), \chi(g_2), \cdots, \chi(g_d)$$

are pairwise distinct, for every non-trivial character $\chi$. This is satisfied when $\Gamma$ is a cyclic group of prime order.

In the rest of this section, let us assume $X = X(\mathbb{Z}_p, \{g_1, g_2, \dots, g_d\})$ for some prime $p$. Let
$$\zeta := e^{2\pi i/p}.$$
We wish to characterize circulant digraphs over $\mathbb{Z}_p$ that admit uniform average vertex mixing. To begin, we prove the following easier direction.

**4.3.4 Lemma.** *Let $p$ be a prime. Let $X$ be a circulant digraph over $\mathbb{Z}_p$ with connection set $\{g_1, g_2, \dots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. If the connection set of $X$ is fixed by some non-trivial automorphism of $\mathbb{Z}_p$, then there is an initial state for which the average probability distribution is not uniform over the vertices.*

*Proof.* Suppose the connection set is invariant under multiplication by $k$, for some $k \in \{2, 3, \cdots, p-1\}$. Let $\chi$ be the character of $\mathbb{Z}_p$ that sends vertex $u$ to $\zeta^u$, and let $\phi$ be the character that sends $u$ to $\zeta^{ku}$. Then there is a permutation $P$ such that
$$P\Lambda_\chi P^T = \Lambda_\phi.$$
If $y$ is an eigenvector for $\Lambda_\chi G$ with eigenvalue $\alpha$, then $Py$ is an eigenvector for $\Lambda_\phi G$ with eigenvalue $\alpha$. By Lemma 4.1.2, both $y \otimes \chi$ and $Py \otimes \phi$ are eigenvectors for $U$ with eigenvalue $\alpha$. Choose $y$ such that
$$(y \otimes \chi + Py \otimes \phi)(y \otimes \chi + Py \otimes \phi)^*$$
has trace one; denote this state by $\rho_0$.

Now let $S$ be the set of outgoing arcs of some vertex $u$. By Theorem 3.2.3, the average probability on $S$, given initial state $\rho_0$, is
$$\begin{aligned} d\sum_r \langle F_r\rho_0 F_r, \rho_S\rangle &= d\langle \rho_0, \rho_S\rangle \\ &= (y \otimes \chi + Py \otimes \phi)^*(I \otimes E_{uu})(y \otimes \chi + Py \otimes \phi) \\ &= 2|y|^2 + 2\mathrm{Re}\left(\langle y, Py\rangle e^{2\pi i(k-1)u/p}\right) \end{aligned}$$
Since $p$ is a prime, the last line cannot be the same for all vertices $u$. □

What about the converse? While we are not able to answer this question in general, we do have the characterization for $d = 2$ and $d = 3$. Some of our techniques may be generalized to circulant digraphs with larger valency.

For $k = 1, 2, \cdots p-1$, define
$$f_k(x) := \frac{1}{x - \zeta^{kg_1}} + \cdots + \frac{1}{x - \zeta^{kg_d}} - \frac{d}{2x}.$$

**4.3.5 Theorem.** *Let $p$ be a prime. Let $X$ be a circulant digraph over $\mathbb{Z}_p$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. The eigenvalues of $U$ are $1$, $-1$, and the set of $\alpha$ such that $f_k(-\alpha^{-1}) = 0$ for some $k = 1, 2, \cdots, p-1$.*

*Proof.* We apply Theorem 4.2.2 to find the eigenvalues of $U$. Fix a non-trivial character $\chi$ of $\mathbb{Z}_p$. Then $\chi(g_j) = \zeta^{kg_j}$ for some $k = 1, 2, \cdots, p-1$. Since $p$ is a prime, $\chi(g_j)$ is distinct over the connection set, so all eigenvalues of $\Lambda_\chi G$ are of the first type in Theorem 4.2.2. The relation between these eigenvalues and the roots of $f_k(x)$ follows from a simple transformation. □

**4.3.6 Corollary.** *Let $p$ be a prime. Let $X$ be a circulant digraph over $\mathbb{Z}_p$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. For $k = 1, 2, \cdots, p-1$, the function $f_k(x)$ has $d$ distinct roots.* □

By manipulating $f_k(x)$, we find an algebraic relation between the eigenvalues of $U$ and those of $X$. That is, each eigenvalue of $U$, other than $\pm 1$, satisfies a polynomial whose coefficients are the eigenvalues of $X$.

**4.3.7 Theorem.** *Let $p$ be a prime. Let $X$ be a circulant digraph over $\mathbb{Z}_p$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. Let $\theta_0, \theta_1, \ldots, \theta_{p-1}$ be the eigenvalues of $X$. The eigenvalues of $U$ are $1$, $-1$, and the set of $\alpha$ such that*

$$\frac{d}{2} = \frac{\theta_0^{\sigma_k} + \theta_1^{\sigma_k}(-\alpha) + \cdots + \theta_{p-1}^{\sigma_k}(-\alpha)^{p-1}}{1 - (-\alpha)^p},$$

*for some $\sigma_k$ in the Galois group $\operatorname{Aut}(\mathbb{Q}(\zeta)/\mathbb{Q})$.*

*Proof.* Let $\alpha \notin \{-1, 1\}$ be an eigenvalue of $U$. Let $\beta = -\alpha$. By Theorem 4.3.5, we have $f_k(\beta) = 0$ for some $k = 1, 2, \cdots, p-1$. Thus,

$$\begin{aligned} \frac{d}{2} &= \sum_{j=1}^{d} \frac{1}{1 - \zeta^{kg_j}\beta} \\ &= \sum_{j=1}^{d} (1 + (\zeta^{kg_j}\beta) + (\zeta^{kg_j}\beta)^2 + \cdots) \end{aligned}$$

$$= \sum_{j=1}^{d} \frac{1 + \zeta^{kg_j}\beta + \cdots + (\zeta^{kg_j}\beta)^{p-1}}{1-\beta^p}$$
$$= \frac{1}{1-\beta^p}\left(p - 1 + \left(\sum_{j=1}^{d} \zeta^{g_j}\right)^{\sigma_k} \beta + \cdots + \left(\sum_{j=1}^{d} \zeta^{(p-1)g_j}\right)^{\sigma_k} \beta^{p-1}\right).$$

Note that for $\ell = 0, 1, 2 \cdots, p-1$,

$$\sum_{j=1}^{d} \zeta^{\ell g_j}$$

is precisely the $\ell$-th eigenvalue $\theta_\ell$ of $X$. □

Both Theorem 4.3.5 and Theorem 4.3.7 give formulas for the eigenvalues of $U$. Our next goal is to derive a sufficient condition, based on Theorem 4.3.5, for uniform average vertex mixing to happen. Define

$$q_k(x) := (x - \zeta^{kg_1}) \cdots (x - \zeta^{kg_d}).$$

Note that $x$ is a root of $f_k(x)$ if and only if it is a root of

$$h_k(x) := dq_k(x) - 2xq_k'(x).$$

The following is a sufficient condition for uniform average vertex mixing to occur.

**4.3.8 Lemma.** *Let $p$ be a prime. Let $X$ be a circulant digraph over $\mathbb{Z}_p$ with connection set $\{g_1, g_2, \ldots, g_d\}$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. If for any $k = 2, 3, \cdots, p-1$, the polynomials $h_1(x)$and $h_k(x)$ are coprime over $\mathbb{C}[x]$, then $U$ admits uniform average vertex mixing.*

*Proof.* Recall from Corollary 4.3.6 that each of $h_1(x), \cdots, h_{p-1}(x)$ has $d$ distinct roots. Thus, if $h_1(x), \cdots, h_{p-1}(x)$ are pairwise coprime over $\mathbb{C}[x]$, then the only non-simple eigenvalue of $U$ is $-1$ with multiplicity $d-1$, and so uniform average vertex mixing occurs. Since the set

$$\{h_1(x), \cdots, h_{p-1}(x)\}$$

is closed under the action of the Galois group $\mathrm{Aut}(\mathbb{Q}(\zeta)/\mathbb{Q})$, it suffices to assume that $h_1(x)$ and $h_k(x)$ are coprime over $\mathbb{C}[x]$, for $k = 2, 3, \cdots, d$. □

We apply the above criterion to $X$ with $d = 2$. This is not the most exciting quantum walk, as the $2 \times 2$ Grover coin is simply a permutation matrix. However, the result gives some hint on the condition we should impose on the connection set.

**4.3.9 Theorem.** *Let $p$ be a prime and $X$ a 2-regular circulant digraph over $\mathbb{Z}_p$. Let $U$ be the transition matrix of a shunt-decomposition Grover walk on $X$. Then $U$ admits uniform average vertex mixing if and only if the connection set is not inverse closed, that is, $X$ is not a graph.*

*Proof.* Let $X = X(\mathbb{Z}_p, \{g_1, g_2\})$. Note that

$$2q_k(x) - 2xq_k'(x) = 0$$

if and only if

$$x^2 = \zeta^{k(g_1+g_2)}.$$

Hence $f_1(x) = f_k(x)$ if and only if $g_1 + g_2 = p$. □

## 4.4 3-Regular Circulants

We generalize our last theorem to 3-regular circulant digraphs on $p$ vertices, for any prime $p \geq 5$. The analysis becomes much more complicated now. To start, we need the following result on cyclotomic integers.

**4.4.1 Lemma.** *Let $m \in \mathbb{Z}$ and let $p \geq 5$ be a prime. If $m$ divides a cyclotomic integer*

$$\sum_{j=0}^{p-1} a_j \zeta^j,$$

*then*

$$a_0 \equiv a_1 \equiv \cdots \equiv a_{p-1} \pmod{m}.$$

*Proof.* The expression

$$\sum_{j=0}^{p-1} a_j \zeta^j$$

of an element in $\mathbb{Z}[\zeta]$ is unique up to summing integer multiples of

$$1 + \zeta + \cdots + \zeta^{p-1}.$$

□

Next, note that when $d = 3$,

$$h_1(x) = 3x^3 - s_1x^2 - s_2x + 3s_3,$$

where $s_1$, $s_2$, and $s_3$ are elementary symmetric functions in $\zeta^{g_1}$, $\zeta^{g_2}$ and $\zeta^{g_3}$:

$$s_1 = \sum_{j=1}^{3} \zeta^{g_j}, \quad s_2 = \sum_{1 \le j < \ell \le 3} \zeta^{g_j + g_\ell}, \quad s_3 = \zeta^{g_1+g_2+g_3}.$$

Similarly, fixing some $k \in \{2, 3, \cdots, p-1\}$, we can write

$$h_k(x) = 3x^3 - t_1x^2 - t_2x + 3t_3,$$

where $t_1$, $t_2$, and $t_3$ are elementary symmetric functions in $\zeta^{kg_1}$, $\zeta^{kg_2}$ and $\zeta^{kg_3}$.

The *resultant* of two polynomials is the determinant of their Sylvester matrix. Given two polynomials over an integral domain, their resultant is zero if and only if they have a common root.

**4.4.2 Lemma.** *Let $p \ge 5$ be a prime. Let $g_1$, $g_2$ and $g_3$ be three distinct elements in $\mathbb{Z}_p$. Let $s_1$, $s_2$ and $s_3$ be the elementary symmetric functions in $\zeta^{g_1}$, $\zeta^{g_2}$ and $\zeta^{g_3}$. For any $k \in \{2, 3, \cdots, p-1\}$, let $t_1$, $t_2$ and $t_3$ be the elementary symmetric functions in $\zeta^{kg_1}$, $\zeta^{kg_2}$ and $\zeta^{kg_3}$. Let*

$$h_1(x) = 3x^3 - s_1x^2 - s_2x + 3s_3,$$

*and*

$$h_k(x) = 3x^3 - t_1x^2 - t_2x + 3t_3.$$

*If $h_1(x)$ and $h_k(x)$ share a root, then we have the equality*

$$s_1t_2 = s_2t_1$$

*in $\mathbb{Z}_3[\zeta]$.*

*Proof.* The resultant of $h_1(x)$ and $h_k(x)$ is an integer multiple of

$$s_3t_3(s_1 - t_1)(\overline{s_1 - t_1})(s_1t_2 - s_2t_1) + 3\gamma$$

for some $\gamma \in \mathbb{Z}[\zeta]$. If $h_1(x)$ and $h_k(x)$ share a root, then their resultant is zero and so 3 divides

$$(s_1 - t_1)(\overline{s_1 - t_1})(s_1t_2 - s_2t_1)$$

in $\mathbb{Z}[\zeta]$. By Lemma 4.4.1, the expression $(s_1 - t_1)(\overline{s_1 - t_1})(s_1 t_2 - s_2 t_1)$ is a polynomial in $\zeta$ whose coefficients are congruent to each other modulo 3. Suppose

$$s_1 t_2 - s_2 t_1 = \sum_{j=0}^{p-1} a_j \zeta^j.$$

Let $a$ be the vector of the coefficients, that is,

$$a = \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_{p-1} \end{pmatrix}.$$

We derive conditions $a$ needs to satisfy.

Let $P$ be the $p \times p$ circulant permutation matrix

$$P := \begin{pmatrix} 0 & 1 & 0 & \cdots & 0 \\ 0 & 0 & 1 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 1 \\ 1 & 0 & 0 & \cdots & 0 \end{pmatrix}.$$

Define

$$Q = P^{g_1} + P^{g_2} + P^{g_3} - P^{kg_1} - P^{kg_2} - P^{kg_3}.$$

Then

$$(s_1 - t_1)(\overline{s_1 - t_1})(s_1 t_2 - s_2 t_1)$$

is a polynomial in $\zeta$ with entries of $Q^T Q a$ as coefficients. Thus $Q^T Q a$ is a constant vector over $\mathbb{Z}_3$. On the other hand, both the rows and the columns of $Q$ generate the same cyclic code over $\mathbb{Z}_3$ with dimension $p-1$, whose dual code is generated by $\mathbf{1}$. Therefore,

$$Q^T Q a \equiv 0 \pmod 3.$$

It follows that $Qa \equiv 0 \pmod 3$, and so $a$ must be a constant vector over $\mathbb{Z}_3$. Note that there are no more than 18 non-zero entries in $a$, so for $p \geq 19$, we must have $a \equiv 0 \pmod 3$. The cases where $p < 19$ can be easily verified by computation. □

**4.4.3 Lemma.** *Let $p \geq 5$ be a prime. Let $g_1$, $g_2$ and $g_3$ be three distinct elements in $\mathbb{Z}_p$. Let $s_1$, $s_2$ and $s_3$ be the elementary symmetric functions in $\zeta^{g_1}$, $\zeta^{g_2}$ and $\zeta^{g_3}$. For any $k \in \{2, 3, \cdots, p-1\}$, let $t_1$, $t_2$ and $t_3$ be the elementary symmetric functions in $\zeta^{kg_1}$, $\zeta^{kg_2}$ and $\zeta^{kg_3}$. Let*

$$h_1(x) = 3x^3 - s_1x^2 - s_2x + 3s_3,$$

*and*

$$h_k(x) = 3x^3 - t_1x^2 - t_2x + 3t_3.$$

*If $h_1(x)$ and $h_2(x)$ share a root, then the set $\{g_1, g_2, g_3\}$ is fixed by some non-trivial automorphism of $\mathbb{Z}_p$.*

*Proof.* The case where $p = 5$ can be easily verified. Let $p \geq 7$. Suppose $h_1(x)$ and $h_2(x)$ share a root. By Lemma 4.4.2,

$$s_1t_2 - s_2t_1$$

is a polynomial $\psi(\zeta)$ in $\zeta$ whose coefficients are all divisible by 3. For notational ease, let

$$z_j := \zeta^{g_j}.$$

We expand $s_1t_2$ and $s_2t_1$:

$$\begin{aligned} s_1t_2 = & z_1z_2^kz_3^k + z_1^kz_2z_3^k + z_1^kz_2^kz_3 && (4.4.1)\\ & + z_1^{k+1}z_2^k + z_2^{k+1}z_3^k + z_1^kz_3^{k+1} && (4.4.2)\\ & + z_1^{k+1}z_3^k + z_1^kz_2^{k+1} + z_2^kz_3^{k+1}. && (4.4.3) \end{aligned}$$

$$\begin{aligned} s_2t_1 = & z_1z_2z_3^k + z_1z_2^kz_3 + z_1^kz_2z_3 && (4.4.4)\\ & + z_1^{k+1}z_2 + z_2^{k+1}z_3 + z_1z_3^{k+1} && (4.4.5)\\ & + z_1^{k+1}z_3 + z_1z_2^{k+1} + z_2z_3^{k+1}. && (4.4.6) \end{aligned}$$

Consider two cases.

(i) All coefficients in $\psi(\zeta)$ are zero. Then there is a bijection between the nine terms in Lines (4.4.1), (4.4.2), (4.4.3) and the nine terms in Lines (4.4.4), (4.4.5), (4.4.6). In particular, both sets of terms have the same product. Thus,

$$s_3^{3k+6} = s_3^{6k+3},$$

and so $k = p-1$. Combining this with $s_1t_2 = s_2t_1$, we have $s_1^2 = s_2^2$. Clearly, $s_1 \neq -s_2$ for $p \geq 7$. If $s_1 = s_2$, playing the same product trick shows that $s_3 = 1$. Now ,

$$s_1 = \overline{s_2}s_3 = \overline{s_1},$$

which is impossible.

(ii) Some coefficient in $\psi(\zeta)$ is at least 3. Then at least three of the nine terms in Lines (4.4.1), (4.4.2), (4.4.3) are equal to some value $\beta$.

(a) One of the three terms in Line (4.4.1), say $z_1z_2^kz_3^k$, is equal to $\beta$. Clearly,

$$\beta \notin \{z_1^kz_2z_3^k, z_1^kz_2^kz_3, z_1^{k+1}z_2^k, z_2^{k+1}z_3^k, z_1^{k+1}z_3^k, z_2^kz_3^{k+1}\}.$$

Hence we must have

$$\beta = z_1z_2^kz_3^k = z_1^kz_2^{k+1} = z_1^kz_3^{k+1}. \tag{4.4.7}$$

The last equality implies $k = p-1$, while the second equality implies $z_1^3 = s_3$. Now

$$s_1t_2 = 3\overline{z_1} + \overline{z_1}z_2\overline{z_3} + \overline{z_1}\,\overline{z_2}z_3 + 2\overline{z_2} + 2\overline{z_3}.$$

It is not hard to verify that

$$\overline{z_1}z_2\overline{z_3}, \overline{z_1}\,\overline{z_2}z_3, \overline{z_2}, \overline{z_3}$$

are pairwise distinct. Thus the last four terms on the right hand side of Equation 4.4.7 cannot survive in $s_1t_2 - s_2t_1$, and from the expansion of $s_2t_1$, we must have

$$\overline{z_1}z_2\overline{z_3} + \overline{z_1}\,\overline{z_2}z_3 + 2\overline{z_2} + 2\overline{z_3} = z_1\overline{z_2}z_3 + z_1z_2\overline{z_3} + 2z_2 + 2z_3.$$

Since $p \geq 7$ is a prime, this can only happen when

$$\{\overline{z_1}z_2\overline{z_3}, \overline{z_1}\,\overline{z_2}z_3, \overline{z_2}, \overline{z_3}\} = \{z_1\overline{z_2}z_3, z_1z_2\overline{z_3}, z_2, z_3\}.$$

As a result, both sets have the same product, and so $z_1 = s_3$, which contradicts $z_1^3 = s_3$.

(b) No term in Line (4.4.1) is equal to $\beta$. Suppose without loss of generality that $\beta = z_1^{k+1} z_2^k$. Clearly,

$$\beta \notin \{z_1^{k+1} z_3^k, z_1^k z_2^{k+1}\}.$$

Also, since

$$z_2^k z_3^{k+1} \notin \{z_2^{k+1} z_3^k, z_1^k z_3^{k+1}\},$$

for $\beta$ to appear at least three times in Line (4.4.2) and Line (4.4.3), it must be that

$$\beta = z_1^{k+1} z_2^k = z_2^{k+1} z_3^k = z_1^k z_3^{k+1}. \tag{4.4.8}$$

It is not hard to verify that the remaining six terms in Line (4.4.1) and Line (4.4.3) are pairwise distinct, given Equation 4.4.8. Thus they have to vanish in $s_1 t_2 - s_2 t_1$. Meanwhile,

$$\begin{aligned} s_2 t_1 =& z_1^k z_2 z_3 + z_1 z_2^k z_3 + z_1 z_2 z_3^k \\ &+ z_1^{k+1} z_2 + z_2^{k+1} z_3 + z_1 z_3^{k+1} \\ &+ 3 z_1^{k+1} z_3. \end{aligned}$$

Thus,

$$\begin{aligned} &z_1 z_2^k z_3^k + z_1^k z_2 z_3^k + z_1^k z_2^k z_3 + z_1^{k+1} z_2^k + z_2^{k+1} z_3^k + z_1^k z_3^{k+1} \\ =& z_1^k z_2 z_3 + z_1 z_2^k z + z_1 z_2 z_3^k + z_1^{k+1} z_2 + z_2^{k+1} z_3 + z_1 z_3^{k+1}. \end{aligned}$$

Again, since $p \geq 7$ is a prime, this implies that the products of terms on both sides are equal. Therefore $s_3 = 1$. It follows from Equation (4.4.8) that

$$z_1^{k+2} = z_3^{k-1}, \quad z_2^{k+2} = z_3^{k-1}, \quad z_3^{k+2} = z_2^{k-1}. \tag{4.4.9}$$

Since $k-1$ is coprime to $p$, there exists an integer $\ell$ such that

$$(k-1)\ell \equiv 1 \pmod{p}.$$

Therefore Equation 4.4.9 shows that the connection set is invariant under multiplication by $\ell$ in $\mathbb{Z}_p$. □

We are now ready to characterize 3-regular circulant digraphs on a prime number of vertices that admit uniform average vertex mixing.

**4.4.4 Theorem.** *Let $p$ be a prime. Let $X$ be a 3-regular circulant digraph over $\mathbb{Z}_p$. Then the shunt-decomposition Grover walk on $X$ admits uniform average vertex mixing if and only if its connection set has trivial stabilizer in* $\mathrm{Aut}(\mathbb{Z}_p)$.

*Proof.* Let $X$ be a 3-regular circulant digraph on $p$ vertices. Let $U$ be the transition matrix of the shunt-decomposition Grover walk on $X$. If the connection set is not fixed by any non-trivial automorphism of $\mathbb{Z}_p$, then by Lemma 4.4.3,

$$\gcd(h_1(x), h_k(x)) = 1$$

for all $k = 2, 3, \cdots, p-1$. On the other hand, since

$$\{h_1(x), \cdots, h_{p-1}(x)\}$$

is closed under the action of $\mathrm{Aut}(\mathbb{Q}[\zeta]/\mathbb{Q})$, any rational root $x_0$ of one polynomial must be a common root of the remaining $p-2$ polynomials. Therefore none of $h_1(x), \cdots, h_{p-1}(x)$ has 1 or $-1$ as a root. The result then follows from Theorem 4.3.3. □

## 4.5 Non-Commuting Shunts

Our analysis of shunt-decomposition walks on Cayley digraphs over abelian groups makes a big assumption, that is, all the shunts are induced by the connection set. Consequently, these shunts commute, and so Theorem 4.2.1 applies. However, there are many more shunt-decompositions of a digraph $X$, possibly non-commuting, that are in one-to-one correspondence to the 1-factorizations of $K_2 \times X$. Do we have machinery to deal with walks based on these shunt-decompositions?

Let us first review what we need to analyze a shunt-decomposition walk with commuting shunts: we want a basis of $\mathbb{C}^{nd}$, under which the coin matrix can be written as $C \otimes I$, while the shift matrix can be written as a block matrix where all the $n \times n$ blocks commute. Now, suppose there is another basis of $\mathbb{C}^{nd}$, under which the shift matrix can be written as $P \otimes I$, while the coin matrix can be written as a block matrix where all the $d \times d$ blocks commute. The common eigenvectors of these blocks will determine the eigenvectors of $U$.

**4.5.1 Theorem.** *Let $X$ be a $d$-regular digraph on $n$ vertices. Consider a shunt-decomposition of $X$, where all the shunts have the same cycle structure. Suppose there is some basis of $\mathbb{C}^{nd}$, under which the shift matrix $S$ can be written as*

$$S = P \otimes I,$$

*and the coin matrix $T$ can be written as*

$$T = \sum_{j=1}^{n} \sum_{k=1}^{n} E_{jk} \otimes A_{jk}$$

*where $A_{jk}$'s pairwise commute. Let $U = ST$ be the transition matrix. Let $\chi$ be a common eigenvector for $A_{jk}$'s with*

$$A_{jk}\chi = \lambda_{jk}\chi,$$

*and set*

$$\Lambda := \begin{pmatrix} \lambda_{11} & \cdots & \lambda_{1n} \\ \cdots & \cdots & \cdots \\ \lambda_{n1} & \cdots & \lambda_{nn} \end{pmatrix}.$$

*Then $y \otimes \chi$ is an eigenvector for $U$ with eigenvalue $\alpha$ if and only if $y$ is an eigenvector for $P\Lambda$ with eigenvalue $\alpha$.*

*Proof.* We have

$$\begin{aligned} U(y \otimes \chi) &= (P \otimes I) \left( \sum_{j,k} E_{jk} \otimes A_{jk} \right) (y \otimes \chi) \\ &= \left( \sum_{j,k} \lambda_{jk} P E_{jk} y \right) \otimes \chi \\ &= (P\Lambda y) \otimes \chi \end{aligned}$$

Thus $U(y \otimes \chi) = \alpha(y \otimes \chi)$ if and only if $P\Lambda y = \alpha y$. □

From now on, let $X$ be a $d$-regular digraph on $n$ vertices with a shunt-decomposition:

$$A = P_1 + \cdots + P_d.$$

Suppose there are permutation matrices $Q_1, Q_2, \ldots, Q_d$ such that for $s = 1, 2, \cdots, d$,

$$Q_s^T P_s Q_s = P_1.$$

It is not hard to see that under some basis of $\mathbb{C}^{nd}$, we can write $U$ as

$$U = (P_1^{-1} \otimes I) \left( \sum_{s,t} Q_s^T Q_t \otimes C_{st} E_{st} \right).$$

We may further express the coin matrix in block form.

**4.5.2 Lemma.** *Let $X$ be a digraph with shunt-decomposition*

$$A = P_1 + \cdots + P_d.$$

*Suppose there are permutation matrices $Q_1, \cdots, Q_d$ such that for $s = 1, 2, \cdots, d$,*

$$Q_s^T P_s Q_s = P_1.$$

*For $j, k = 1, 2, \cdots, n$, let*

$$A_{jk} := \sum_{s,t} (Q_s^T Q_t)_{jk} C_{st} E_{st}.$$

*Then the shunt-decomposition $C$-walk on $X$ has transition matrix*

$$U = (P_1^{-1} \otimes I) \left( \sum_{j,k} E_{jk} \otimes A_{jk} \right).$$ □

The formula for $A_{jk}$ can be simplified when $C$ is the Grover coin.

**4.5.3 Lemma.** *Let $X$ be a digraph with shunt-decomposition*

$$A = P_1 + \cdots + P_d.$$

*Suppose there are permutation matrices $Q_1, \cdots, Q_d$ such that for $s = 1, 2, \cdots, d$,*

$$Q_s^T P_s Q_s = P_1.$$

*For $j, k = 1, 2, \cdots, n$, let*

$$A_{jk} = \delta_{jk} \left( \frac{2}{d} - 1 \right) I + \frac{2}{d} \left( \sum_{s \neq t} (Q_s^T Q_t)_{jk} E_{st} \right).$$

*Then the shunt-decomposition Grover walk on $X$ has transition matrix*

$$U = (P_1^{-1} \otimes I) \left( \sum_{j,k} E_{jk} \otimes A_{jk} \right).$$ □

We have found shunt-decompositions for which $A_{jk}$'s commute, with respect to the Grover coin. An example of $K_{3,3}$ is given in Figure 4.1, where arcs with the same color form a shunt. From the figure, it is easy to check that these shunts do not commute; for instance, if the red shunt commutes with the blue shunt, then for any $uv$-walk that consists of a red arc followed by a blue arc, there is a $uv$-walk that consists of a blue arc followed by a red arc. The associated shunt-decomposition Grover walk exhibits an interesting property—there is perfect state transfer from one arc to another at step 4; in fact, $U^4$ is a permutation matrix.

Figure 4.2 gives another shunt-decomposition with non-commuting shunts, for which $U^4$ is also a permutation matrix.

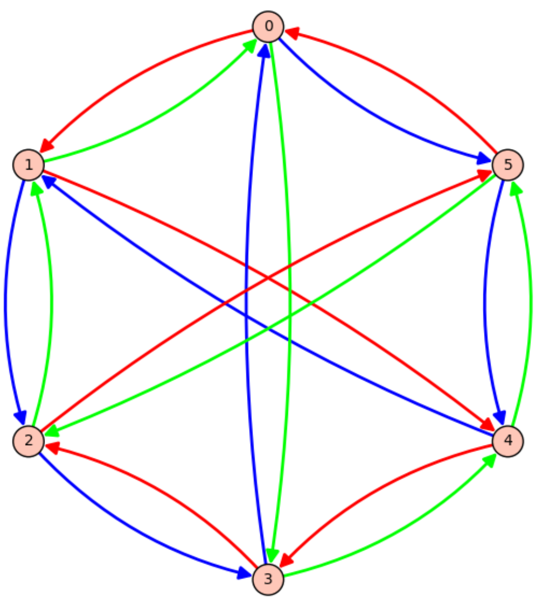



Figure 4.1: A shunt-decomposition of $K_{3,3}$

## 4.6 Infinite Paths

At the end of this chapter, we briefly discuss another approach to shunt-decomposition walks on infinite graphs, based on the paper by Ambainis, Bach, Nayak, Vishwanath, and Watrous [4].

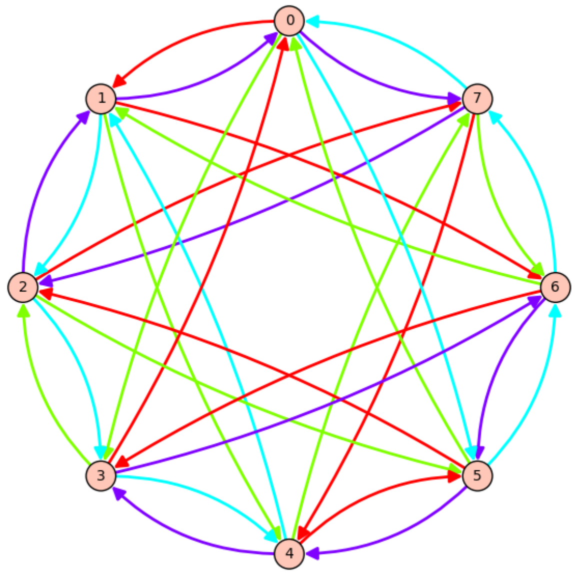



Figure 4.2: A shunt-decomposition of $K_{4,4}$

While a lot has been done since Aharonov et al [2] introduced the shunt-decomposition model, most work focused on presenting numerical results. The first paper with exact analysis was due to Ambainis et al [4], who studied the limiting behavior of a shunt-decomposition Hadamard walk on the infinite path $P_\infty$.

As usual, the quantum walker moves on the arcs of $P_\infty$. The state space can be identified as $\mathbb{C}^{\mathbb{Z}} \otimes \mathbb{C}^2$ (more formally, $\ell_2(\mathbb{C}^{\mathbb{Z}}) \otimes \mathbb{C}^2$). Let

$$H := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$$

be the Hadamard coin. Let $S$ be the linear operator such that

$$S(e_u \otimes e_1) = e_{u+1} \otimes e_1$$

and

$$S(e_u \otimes e_2) = e_{u-1} \otimes e_2.$$

Then the transition operator is

$$U = S(H \otimes I).$$

Given initial state $e_0 \otimes e_1$, let $\Psi(u,k)$ be the coin state on vertex $u$ at time $k$. Ambainis et al [4] derived a recurrence relation for $\Psi(u,k)$:

$$\Psi(u,k+1) = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 0\\ 1 & 1\end{pmatrix}\Psi(u-1,k) + \frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 1\\ 0 & 0\end{pmatrix}\Psi(u+1,k),$$

with initial conditions

$$\Psi(0,0) = \begin{pmatrix}0\\ 1\end{pmatrix}$$

and

$$\Psi(u,0) = \begin{pmatrix}0\\ 0\end{pmatrix},$$

for all $u \neq 0$. Using this recurrence, they proved several properties of the probability distribution, all strikingly different from the classical random walk on $P_\infty$. For example, after $k$ steps, the probability distribution of this Hadamard walk is nearly uniform over the vertices between $-k/\sqrt{2}$ and $k/\sqrt{2}$, while a classical random walker tends to stay at distance $O(\sqrt{k})$ from the origin with high probability. In the presence of absorbing boundaries, the exit probabilities are also in sharp contrast to those of the classical random walk. With one absorbing boundary at vertex 0, the probability that the walker exits to the left is $2/\pi$, and with an additional absorbing boundary at vertex $u$, this probability increases, and approaches $1/\sqrt{2}$ as $u$ goes to infinity. Both probabilities in the classical random walk are 1.

## 4.7 Open Problems

We list some open problems regarding shunt-decomposition walks.

An immediate task is to solve the generalization of Theorem 4.4.4. Numerical experiments suggest that the same characterization may hold for circulant digraphs over $\mathbb{Z}_p$ with higher valency. We leave this problem as a conjecture.

(i) **Conjecture.** Let $p$ be a prime. A circulant digraph on $p$ vertices admits uniform average vertex mixing if and only if its connection set has trivial stabilizer in $\mathrm{Aut}(\mathbb{Z}_p)$.

Note that this characterization does not hold if we replace $\mathbb{Z}_p$ by $\mathbb{Z}_n$, where $n$ is a composite. Even if the digraph has distinct eigenvalues, there might be an initial state for which the average probability distribution is not uniform over $V(X)$; an example is given by $X(\mathbb{Z}_{10}, \{1, 2, 3\})$.

Another direction is to extend the work on non-commuting shunts. For instance, according to Lemma 4.5.3, one may translate the property that $A_{jk}$'s pairwise commute, with respect to the Grover coin, into properties of $Q_1, Q_2, \ldots, Q_d$, and thus properties of the shunts. It is also possible to characterize shunt-decompositions that "interact nicely" with other popular coins, such as the Fourier coin. In general, we would like to understand the following.

(ii) Given a coin $C$ and a shunt-decomposition with non-commuting shunts, how much spectral information can we obtain about $U$?

Finally, we wish to compare walks on the same digraph with different shunt-decompositions. Note that this may include comparing shunt-decomposition walks to arc-reversal walks—for a $d$-regular graph with edge chromatic number $d$, the arc-reversal operator $R$ is indeed a shift operator, obtained from a $d$-edge-coloring. In fact, such a comparison between two models has been done for designing better algorithms. Ambainis et al [5] studied two quantum search algorithms on the 2-dimensional grid with $n$ vertices, one based on the arc-reversal walk, and one on the shunt-decomposition walk. It turns out that the arc-reversal search succeeds in $O(\sqrt{n}\log(n))$ steps, while the shunt-decomposition search takes time $\Omega(n)$. On the other hand, our numerical results in Table 3.1 show that on the same circulant graph, the shunt-decomposition walk may mix faster than the arc-reversal walk. In general, we would like to know what makes a shunt-decomposition walk perform better than the other.

(iii) Given a regular digraph $X$, can we optimize a parameter, such as the mixing time, of quantum walks on $X$ over all possible shunt-decompositions?

# Chapter 5

# Walking on Embeddings

With various transition operators implemented, our quantum walker learns that unitarity is the physics law she cannot violate, while sparseness is the extra property she desires for efficiency. To travel across the entire graph, an ideal transition operator would alternate between two block-diagonal unitary matrices, each partitioning the arcs in some way. Edges, tails, heads, shunts...; all of these have been considered when it comes to dividing the arcs, and familiar models such as arc-reversal walks and shunt-decomposition walks arise from these partitions. Now, what if we group the arcs based on an embedding? The curious walker wonders.

In this chapter, we construct a new quantum walk, called the vertex-face walk, from an orientable embedding of a graph. Once a consistent orientation of the faces is chosen, there is a natural partition of the arcs into facial walks; let $M$ be the associated arc-face incidence matrix. Let $N = D_t^T$ be the arc-tail incidence matrix. The transition matrix of the vertex-face walk is then given by the two reflections about $\operatorname{col}(M)$ and $\operatorname{col}(N)$:

$$U = (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I).$$

Although the vertex-face model has never been studied before, it is closely related to the arc-reversal model. Given an embedding $\mathcal{M}$ of a graph $X$, the *dual graph*, denoted $X^*$, is the graph with faces in $\mathcal{M}$ as vertices, and two vertices are adjacent in $X^*$ if the corresponding faces share an edge in $X$. It turns out that each step of the new walk is equivalent to two steps of the arc-reversal walk, one on the original graph, and one on the dual graph. For another connection to the literature, we remark that the vertex-face walk on $C_n \square C_n$ with a toroidal embedding is equivalent to the quantum walk used in [6], for the spacial search on a 2-dimensional lattice, as we explained in Section 1.3.

We motivate our study on the new walk by asking two questions, which have no satisfactory answers in the existing literature. First, while there is no exact relation between the continuous quantum walk and the discrete quantum walk on the same graph, mathematically one can write any unitary matrix $U$ as

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

for some Hermitian matrix $H$. From this perspective, every discrete quantum walk is a continuous quantum walk on some weighted digraph, with time discretized. What we are interested in is the following problem.

- For which $U$ is $H$ a sparse Hermitian adjacency matrix of a digraph?

The second question concerns the limiting behavior of a class of quantum walks. Unlike classical random walks, quantum walks may be sedentary—the probability that the system stays at the initial state goes to 1 as the size of the graph grows. For continuous quantum walks, Godsil [30] studied large families of strongly regular graphs that tend to "stay at home". We seek discrete analogues.

- Is there a sedentary family of discrete quantum walks?

Once again, these questions can be investigated through spectral analysis of the transition matrix. However, they quickly become intractable when $U$ has too many eigenvalues. In the arc-reversal model, every graph eigenvalue contributes to two eigenvalues of $U$; in the shunt-decomposition model the situation is worse—for each character, there is a modified coin whose spectrum is contained in the spectrum of $U$.

In contrast, the vertex-face model offers some examples with few eigenvalues. In fact, we have the following characterization in terms of the embeddings. It is perhaps surprising that symmetric designs come into play.

(i) The transition matrix has exactly two eigenvalues if and only if every face is bounded by a Hamilton cycle.

(ii) For a circular embedding of a regular graph, the transition matrix has exactly three eigenvalues if and only if the vertex-face incidence structure is a symmetric 2-design. Moreover, any such walk is a discretization of a continuous quantum walk on an oriented graph.

Following these observations, we find two infinite families of embeddings that manifest properties raised by both questions. These families are constructed from regular embeddings, as we define in Section 5.6.

(i) Let $n$ be a prime power. Let $U$ be the transition matrix of the vertex-face walk for a regular embedding of $K_n$. Then there is $\gamma \in \mathbb{R}$ such that
$$U = \exp(\gamma(U^T - U)).$$
Moreover, $U^T - U$ is a scalar multiple of the skew-symmetric adjacency matrix of an oriented graph $Z_n$, which

  (a) has $n(n-1)$ vertices,

  (b) is $(n-2)$-regular, and

  (c) has exactly three eigenvalues: 0 and $\pm i\sqrt{n^2 - 2n}$.

The vertex-face walks for these embeddings form a sedentary family of quantum walks.

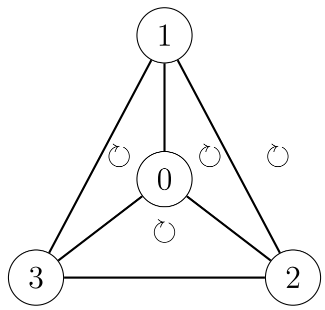
(ii) Let $n$ be a power of 2. Let $\mathcal{M}_n$ be a regular embedding of $K_n$. Let $\psi$ be the covering map from $K_2 \times K_n$ to $K_n$. Let $\mathcal{M}_n'$ be the embedding of $K_2 \times K_n$ whose facial walks are the preimages of the facial walks of $\mathcal{M}_n$. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}_n'$. Then $U$ has exactly four eigenvalues. Moreover, there is $\gamma \in \mathbb{R}$ such that
$$U^2 = \exp(\gamma(U^T - U)),$$
and $U^T - U$ is a scalar multiple of the skew-symmetric adjacency matrix of the double graph of $Z_n$. The vertex-face walks for these embeddings form a sedentary family of quantum walks.

Most results in this chapter can be found in Zhan [67].

## 5.1 Vertex-Face Walk

We introduce the vertex-face walk through an example. Consider the planar embedding $\mathcal{M}$ of $K_4$. As shown in Figure 5.1, since the surface is orientable, we can choose a consistent orientation of the face boundaries. This partitions the arcs of $K_4$ into four groups $\{f_0, f_1, f_2, f_3\}$, called the *facial walks*.

Meanwhile, the arcs can be partitioned into another four groups, each having the same tail. We represent these two partitions by the incidence matrices $M$ and $N$, called the *arc-face incidence matrix* and the *arc-tail incidence matrix*, respectively, in Equation (5.1.1).




Facial walks:

$f_0 = \{(0,1),(1,2),(2,0)\}$
$f_1 = \{(1,3),(3,2),(2,1)\}$
$f_2 = \{(0,2),(2,3),(3,0)\}$
$f_3 = \{(0,3),(3,1),(1,0)\}$

Figure 5.1: A planar embedding of $K_4$

$$M = \begin{array}{c} \\ (0,1) \\ (0,2) \\ (0,3) \\ (1,0) \\ (1,2) \\ (1,3) \\ (2,0) \\ (2,1) \\ (2,3) \\ (3,0) \\ (3,1) \\ (3,2) \end{array} \begin{array}{c} \begin{array}{cccc} f_0 & f_1 & f_2 & f_3 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \end{pmatrix} \end{array} \qquad N = \begin{array}{c} \\ (0,1) \\ (0,2) \\ (0,3) \\ (1,0) \\ (1,2) \\ (1,3) \\ (2,0) \\ (2,1) \\ (2,3) \\ (3,0) \\ (3,1) \\ (3,2) \end{array} \begin{array}{c} \begin{array}{cccc} 0 & 1 & 2 & 3 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \tag{5.1.1}$$

Let $\widehat{M}$ and $\widehat{N}$ be the matrices obtained from $M$ and $N$ by scaling each column to a unit vector; they will be referred to as the *normalized arc-face incidence matrix* and the *normalized arc-tail incidence matrix*. Then $2\widehat{M}\widehat{M}^T - I$ and $2\widehat{N}\widehat{N}^T - I$ are two reflections, and

$$U := (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I).$$

is a unitary matrix. The quantum walk with $U$ as the transition matrix is called the *vertex-face walk* relative to the chosen orientation of $\mathcal{M}$.

This construction can be easily generalized to any orientable embedding $\mathcal{M}$ of a graph $X$. Although $U$ depends on the consistent orientation, there are only two choices—reversing all the arcs in the facial walks of one orientation produces the other. Therefore, if

$$(2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I)$$

is the transition matrix relative to the "clockwise" orientation, then

$$R(2\widehat{M}\widehat{M}^T - I)R(2\widehat{N}\widehat{N}^T - I)$$

is the transition matrix relative to the "counterclockwise" orientation. Here, $R(2\widehat{N}\widehat{N}^T - I)$ determines the arc-reversal walk on $X$. On the other hand, each orientation defines a bijection between the arcs of $X$ and the arcs of its dual graph $X^*$. Under this bijection,

$$R(2\widehat{M}\widehat{M}^T - I)$$

acts as the transition matrix of the arc-reversal walk on the dual graph. Hence, the vertex-face walk can be viewed as a variation of the arc-reversal walk—every other step of the arc-reversal walk on $X$ is replaced by a step on $X^*$.

In this chapter, most of our results are independent of the consistent orientation, so we will simply refer to $U$ as the transition matrix of a vertex-face walk for an embedding, if it is clear from the context.

Naturally, $\mathcal{M}$ gives rise to an embedding of $X^*$ on the same surface, denoted $\mathcal{M}^*$. The following observation on duality is immediate.

**5.1.1 Lemma.** *If $U$ is the transition matrix of a vertex-face walk for the orientable embedding $\mathcal{M}$, then $U^T$ is the transition matrix of the vertex-face walk for $\mathcal{M}^*$.* □

Unless otherwise specified, we will assume that $\mathcal{M}$ is a *circular embedding*, that is, an embedding where every face of $\mathcal{M}$ is bounded by a cycle.

Now we move on to discuss some properties of $U$. For ease of notation, let

$$P := \widehat{M}\widehat{M}^T$$

and

$$Q := \widehat{N}\widehat{N}^T.$$

Note that $P$ is the projection onto vectors constant on each facial walk, and $Q$ is the projection onto vectors constant on arcs leaving each vertex. It is not hard to verify the following.

**5.1.2 Lemma.** *Let $\mathcal{M}$ be a circular embedding of a graph $X$. Let $\widehat{M}$ and $\widehat{N}$ be the associated normalized arc-face incidence matrix and normalized arc-tail incidence matrix, respectively. Let*

$$P = \widehat{M}\widehat{M}^T, \quad Q = \widehat{N}\widehat{N}^T.$$

*Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$, that is,*

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

*For any arc $(u, v)$ of $X$, let $f_{uv}$ denote the facial walk using $(u, v)$.*

*(i) The projections $P$ and $Q$ are doubly stochastic, and so*

$$U\mathbf{1} = U^T\mathbf{1} = \mathbf{1}.$$

*(ii) For two arcs $(a, b)$ and $(u, v)$,*

$$P_{(a,b),(u,v)} = \begin{cases} \dfrac{1}{\deg(f_{uv})}, & \text{if } f_{ab} = f_{uv}. \\ 0, & \text{otherwise.} \end{cases},$$

*and*

$$Q_{(a,b),(u,v)} = \begin{cases} \dfrac{1}{\deg(u)}, & \text{if } a = u. \\ 0, & \text{otherwise.} \end{cases}$$

*(iii) For two arcs $(a, b)$ and $(u, v)$,*

$$(PQ)_{(a,b),(u,v)} = (QP)_{(u,v),(a,b)} = \begin{cases} \dfrac{1}{\deg(u)\deg(f_{ab})}, & \text{if } u \in f_{ab}. \\ 0, & \text{otherwise.} \end{cases}$$

*(iv) For two faces $f$ and $h$,*

$$(\widehat{M}^T Q \widehat{M})_{f,h} = \frac{1}{\sqrt{\deg(f)\deg(h)}} \sum_{u \in f \cap h} \frac{1}{\deg(u)}.$$

*For two vertices $u$ and $v$,*

$$(\widehat{N}^T P \widehat{N})_{u,v} = \frac{1}{\sqrt{\deg(u)\deg(v)}} \sum_{f: u,v \in f} \frac{1}{\deg(f)}.$$ □

The above lemma allows us to write out the entries of $U$ explicitly. Moreover, if either $X$ or $X^*$ is regular, we have a simple expression for $\mathrm{tr}(U)$.

**5.1.3 Lemma.** *Let $\mathcal{M}$ be an orientable embedding of $X$ with $n$ vertices, $\ell$ edges and $s$ faces. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$. If either $X$ or $X^*$ is regular, then*

$$\mathrm{tr}(U) = 2\left(\frac{ns}{\ell} - (n + s - \ell)\right).$$

*Proof.* Let $\widehat{M}$ and $\widehat{N}$ be the normalized arc-face incidence matrix and normalized arc-tail incidence matrix for $\mathcal{M}$, respectively. Let

$$P = \widehat{M}\widehat{M}^T, \quad Q = \widehat{N}\widehat{N}^T.$$

We have

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

From (iii) in Lemma 5.1.2 we see that

$$\begin{aligned}\mathrm{tr}(PQ) &= \sum_{(u,v)} \frac{1}{\deg(u)} \frac{1}{\deg(f_{uv})} \\ &= \sum_{f} \frac{1}{\deg(f)} \sum_{u \in f} \frac{1}{\deg(u)}.\end{aligned}$$

If $X$ is $d$-regular, then

$$\mathrm{tr}(PQ) = \frac{s}{d} = \frac{ns}{2\ell}.$$

Hence

$$\begin{aligned}\mathrm{tr}(U) &= 4\,\mathrm{tr}(PQ) - 2\,\mathrm{tr}(P) - 2\,\mathrm{tr}(Q) - \mathrm{tr}(I) \\ &= 2\frac{ns}{\ell} - 2(\mathrm{rk}(P) + \mathrm{rk}(Q) - 2\ell) \\ &= 2\left(\frac{ns}{\ell} - (n + s - \ell)\right).\end{aligned}$$

The case where $X^*$ is regular follows from duality. □

A quantum walk is *reducible* if $U$ is permutation similar to some block-diagonal matrix. In this case, the walk can be decomposed as two or more independent walks in subsystems. A bit of thought reveals that a vertex-face walk is irreducible if and only if the join of the arc-face partition and the arc-tail partition is the trivial partition, that is, the partition with only one class. Using this, we prove that whenever $X$ is connected, any vertex-face walk on $X$ is irreducible. In fact, something stronger about the aforementioned partitions is true.

**5.1.4 Lemma.** *Let $\mathcal{M}$ be an orientable embedding of a connected graph $X$. Let $\pi_1$ and $\pi_2$ be the arc-face partition and the arc-tail partition of $\mathcal{M}$. Then the meet $\pi_1 \wedge \pi_2$ is the discrete partition, and the join $\pi_1 \vee \pi_2$ is the trivial partition.*

*Proof.* First of all, since every face is bounded by a cycle, no two arcs sharing the tail are contained in the same facial walk, so each class in $\pi_1 \wedge \pi_2$ contains only one element. Therefore, $\pi_1 \wedge \pi_2$ is the discrete partition. Next, due to the connectedness of $X$, between any two vertices $v_0$ and $v_k$ there is a path, say

$$v_0, v_1, \ldots, v_k.$$

Consider the first two arcs $(v_0, v_1)$ and $(v_1, v_2)$. If they belong to the same facial walk, then they are in the same class of $\pi_1 \vee \pi_2$. Otherwise, there is an arc $(v_1, w_1)$ that is in the same facial walk as $(v_0, v_1)$. Thus, all outgoing arcs of $v_1$, including $(v_1, v_2)$, are in the same class of $\pi_1 \vee \pi_2$ as $(v_0, v_1)$. Proceeding in this fashion, we see that all arcs in the path belong to the same class of $\pi_1 \vee \pi_2$. □

**5.1.5 Corollary.** *Any vertex-face walk on a connected graph is irreducible.* □

In the rest of this chapter, unless otherwise specified, we will assume $X$ is connected, in addition to that $\mathcal{M}$ is circular.

## 5.2 Spectral Decomposition

Similar to the arc-reversal walk, the vertex-face walk arises from two reflections, so all the results in Section 2.3 apply. In particular, the spectrum of $U$ depends largely on an incidence matrix, which relates the vertices and the faces of an embedding.

Consider a circular embedding $\mathcal{M}$ with $n$ vertices, $\ell$ edges and $s$ faces on an orientable surface of genus $g$. A vertex is incident to a face if it is incident to an edge that is contained in the face. Let $B$, $C$ and $D$ be the *vertex-edge incidence matrix*, the *vertex-face incidence matrix*, and the *face-edge incidence matrix*, respectively. Since every face is bounded by a cycle, we have the following two expressions for $C$.

**5.2.1 Lemma.** *Let $\mathcal{M}$ be a circular embedding of a connected graph $X$. Let $B$, $C$ and $D$ be the vertex-edge incidence matrix, the vertex-face incidence matrix, and the face-edge incidence matrix, respectively. Then*

$$C = BD^T = N^T M. \qquad \square$$

We also define

$$\widehat{C} := \widehat{N}^T \widehat{M},$$

and call it the *normalized vertex-face incidence matrix*. By Lemma 2.3.4, the eigenvalues of $\widehat{C}\widehat{C}^T$ lie in $[0, 1]$. Further, those that are strictly between 0 and 1 contribute fully to the non-real eigenvalues of $U$, while 0 and 1 contribute partially to the real eigenvalues of $U$.

**5.2.2 Theorem.** *Let $X$ be a connected graph with $\ell$ edges. Let $\mathcal{M}$ be a circular embedding of $X$ onto an orientable surface of genus $g$. Let $\widehat{M}$ and $\widehat{N}$ be the associated normalized arc-face incidence matrix and normalized arc-tail incidence matrix, respectively. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$, that is,*

$$U = (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I).$$

*The 1-eigenspace of $U$ is*

$$(\operatorname{col}(\widehat{M}) \cap \operatorname{col}(\widehat{N})) \oplus (\ker(\widehat{M}^T) \cap \ker(\widehat{N}^T))$$

*with dimension $\ell + 2g$. Moreover, the first subspace is 1-dimensional.*

*Proof.* Note that any vector lying in $\operatorname{col}(M) \cap \operatorname{col}(N)$ must be constant over the arcs leaving each vertex, as well as constant on the arcs used by each face. Since $X$ is connected, this vector is constant everywhere. Now the structure and multiplicity of the 1-eigenspace follow from Lemma 2.3.5 and Euler's formula

$$n - \ell + s = 2 - 2g. \qquad \square$$

**5.2.3 Theorem.** *Let $\mathcal{M}$ be a circular embedding of a connected graph $X$ with $n$ vertices and $s$ faces. Let $\widehat{M}$ and $\widehat{N}$ be the associated normalized arc-face incidence matrix and normalized arc-tail incidence matrix, respectively. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$, that is,*

$$U = (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I).$$

*Let $\widehat{C}$ be the normalized vertex-face incidence matrix. The $(-1)$-eigenspace for $U$ is*

$$\widehat{M}\ker(\widehat{C}) \oplus \widehat{N}^T \ker(\widehat{C}^T)$$

*with dimension*

$$n + s - 2\,\mathrm{rk}(\widehat{C}).$$

*Proof.* This follows from Lemma 2.3.6. □

**5.2.4 Theorem.** *Let $\mathcal{M}$ be a circular embedding of a connected graph $X$. Let $\widehat{M}$ and $\widehat{N}$ be the associated normalized arc-face incidence matrix and normalized arc-tail incidence matrix, respectively. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$, that is,*

$$U = (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I).$$

*Let $\widehat{C}$ be the normalized vertex-face incidence matrix. The multiplicities of the non-real eigenvalues of $U$ sum to $2\,\mathrm{rk}(\widehat{C}) - 2$. Let $\mu \in (0,1)$ be an eigenvalue of $\widehat{C}\widehat{C}^T$. Choose $\theta$ with $\cos(\theta) = 2\mu - 1$. The map*

$$y \mapsto (\cos(\theta) + 1)\widehat{N}y - (e^{i\theta} + 1)\widehat{M}\widehat{C}^T y$$

*is an isomorphism from the $\mu$-eigenspace of $\widehat{C}\widehat{C}^T$ to the $e^{i\theta}$-eigenspace of $U$, and the map*

$$y \mapsto (\cos(\theta) + 1)\widehat{N}y - (e^{-i\theta} + 1)\widehat{M}\widehat{C}^T y$$

*is an isomorphism from the $\mu$-eigenspace of $\widehat{C}\widehat{C}^T$ to the $e^{-i\theta}$-eigenspace of $U$.*

*Proof.* This follows from Lemma 2.3.7 and that

$$\dim(\mathrm{col}(M) \cap \mathrm{col}(N)) = 1.$$ □

After normalization, we obtain an explicit formula for the eigenprojection of each non-real eigenvalue of $U$.

**5.2.5 Corollary.** *Let $\mathcal{M}$ be a circular embedding of a connected graph $X$. Let $\widehat{M}$ and $\widehat{N}$ be the associated normalized arc-face incidence matrix and normalized arc-tail incidence matrix, respectively. Let*

$$P = \widehat{M}\widehat{M}^T, \quad Q = \widehat{N}\widehat{N}^T.$$

*Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$, that is,*

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

*Let $\widehat{C}$ be the normalized vertex-face incidence matrix. Let $\mu \in (0, 1)$ be an eigenvalue of $\widehat{C}\widehat{C}^T$. Choose $\theta$ such that $\cos(\theta) = 2\mu - 1$. Let $E_\mu$ be the orthogonal projection onto the $\mu$-eigenspace of $\widehat{C}\widehat{C}^T$. Set*

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

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

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

## 5.3 Hamiltonian

We digress a bit to talk about continuous quantum walks, which evolve quite differently from their discrete counterparts. Given a digraph $Z$ with a Hermitian adjacency matrix $H$, a continuous quantum walk on $Z$ is determined by the transition matrix

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

Physicists refer to $H$ as the *Hamiltonian* of the quantum walk. If $Z$ is undirected, two common choices for the Hamiltonian are the adjacency matrix and the Laplacian matrix of $Z$. If $Z = (V, \mathcal{A})$ is an oriented graph with adjacency matrix $A$, then we can take $H = i(A - A^T)$; in this case, $U(t)$ is actually the continuous quantum walk on the weighted digraph

$$(V, \mathcal{A} \cup \{(u, v) : (v, u) \in \mathcal{A}\}),$$

whose arc $(u, v)$ receives weight $i$ if $(u, v) \in \mathcal{A}$, and $-i$ otherwise.

For years people have spent efforts on understanding the connection between continuous and discrete quantum walks. However, since they do not have the same state space to start with, the correspondence, if any, is not as direct as that between continuous and discrete random walks. While exact relation is not feasible, Childs [15] showed that, up to desired precision, the Hamiltonian of a continuous quantum walk can be simulated using a series of discrete quantum walks, based on Szegedy's model [59].

We study the connection from a different angle. Every unitary matrix $U$ can be expressed as

$$U = \exp(iH)$$

for some Hermitian matrix $H$. Although the choice of $H$ is not unique, we can pick one in a canonical way: if $U$ has spectral decomposition

$$U = \sum_r \alpha_r F_r,$$

then we define the *Hamiltonian* of $U$ to be

$$H := -i \sum_r \log(\alpha_r) F_r,$$

where $-\pi < -i\log(\alpha_r) \leq \pi$ for all $\alpha_r$. Thus, a discrete quantum walk on a digraph with $m$ arcs is equivalent to a continuous quantum walk on a weighted digraph on $m$ vertices, with integer time steps.

If $U$ is a unitary matrix with Hamiltonian $H$, then the *$H$-weighted digraph* is the underlying digraph $Z$ of $H$, together with the weight $H_{u,v}$ on the arc $(u, v)$. Most likely, the $H$-weighted digraph is nearly complete with many weights. A question then arises: for which $U$, is $H$ sparse with few distinct entries?

The answer clearly depends on the interplay of eigenvalues and eigenprojections of $U$. We seek examples in the vertex-face model. Since $U$ is real, its spectrum is closed under complex conjugation, so an alternative expression for the Hamiltonian is

$$H = \pi F_{-1} - \sum_{r:0<-i\log(\alpha_r)<\pi} i\log(\alpha_r)(F_r - F_r^T).$$

Using Corollary 5.2.5, we can write out the second term purely in terms of the spectral decomposition of $\widehat{C}\widehat{C}^T$.

**5.3.1 Lemma.** *Let $\mathcal{M}$ be a circular embedding of a connected graph $X$. Let $\widehat{M}$ and $\widehat{N}$ be the associated normalized arc-face incidence matrix and normalized arc-tail incidence matrix, respectively. Let*

$$P = \widehat{M}\widehat{M}^T, \quad Q = \widehat{N}\widehat{N}^T.$$

*Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$, that is,*

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

*Let $\widehat{C}$ be the normalized vertex-face incidence matrix. For each eigenvalue $\mu \in (0,1)$ of $\widehat{C}\widehat{C}^T$ with eigenprojection $E_\mu$, let $\theta \in (0,\pi)$ be such that $\cos(\theta) = 2\mu - 1$. Then the Hamiltonian of $U$ is*

$$H = \pi F_{-1} + i \sum_{\mu \in (0,1)} \frac{2\theta}{\sin(\theta)} (\widehat{N} E_\mu \widehat{N}^T P - P \widehat{N} E_\mu \widehat{N}^T),$$

*where the sum is taken over all eigenvalues $\mu$ of $\widehat{C}\widehat{C}^T$ in $(0,1)$.* □

## 5.4 Few Eigenvalues

Regular graphs with few eigenvalues, such as complete graphs and strongly regular graphs, were studied at the early age of continuous quantum walks since their spectral decompositions are manageable. For the same reason, we would like to start our study on Hamiltonians with transition matrices that have few eigenvalues.

For the rest of this section, assume $\mathcal{M}$ is a circular orientable embedding of some $d$-regular graph $X$ with $n$ vertices, $\ell$ edges and $s$ faces. In this case, the normalized vertex-face incidence matrix $\widehat{C}$ is simply a multiple of $C$. Let $U$ be the transition matrix of the vertex-face walk relative to some consistent orientation of $\mathcal{M}$. We characterize $\mathcal{M}$ for which $U$ has two or three eigenvalues.

**5.4.1 Theorem.** *Let $U$ be the transition matrix of a vertex-face walk for a circular embedding of a connected graph. Then $U$ has exactly two eigenvalues if and only if each face boundary is a Hamilton cycle.*

*Proof.* Suppose $U$ has exactly two eigenvalues. Then they must be 1 and $-1$. Since there is no non-real eigenvalue, Theorem 5.2.4 tells us that

$$\operatorname{rk}(C) = 1.$$

Thus each facial cycle must visit all vertices. For the converse, simply note that if $\operatorname{rk}(C) = 1$, then

$$n + s - 2\operatorname{rk}(C) \geq 1,$$

so $-1$ must be an eigenvalue. □

The toroidal embedding of $K_{3,3}$ in Figure 5.2 is an example of circular embeddings where every face visits every vertex. While this type of embeddings are interesting on their own, the quantum walks they generate are less exciting, since they all have period two.

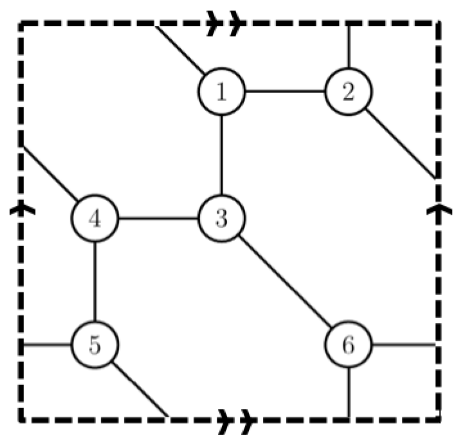



Figure 5.2: $K_{3,3}$ embedded on the torus

The next case is when $U$ has exactly three eigenvalues—one real and two complex.

**5.4.2 Theorem.** *Let $X$ be a connected $d$-regular graph on $n$ vertices. Let $U$ be the transition matrix of a vertex-face walk for a circular embedding of $X$. Then $U$ has exactly three eigenvalues if and only if the vertex-face incidence structure form a symmetric 2-design with parameters*

$$\left(n, d, \frac{(d-1)d}{n-1}\right).$$

*Moreover, if $U$ has exactly three eigenvalues, then* *(i) the eigenvalues are* 1 *and* $e^{\pm i\theta}$, *where*

$$\cos(\theta) = \frac{2(n-d)}{d(n-1)} - 1;$$

*(ii) neither* $X$ *nor* $X^*$ *is bipartite.*

*Proof.* We prove one direction of the first statement. Suppose $U$ has exactly three eigenvalues. Then $-1$ cannot be one of them. By Theorem 5.2.3, we need

$$2\,\mathrm{rk}(C) = n + s.$$

On the other hand,

$$\mathrm{rk}(C) \leq \min\{\mathrm{rk}(N), \mathrm{rk}(M)\} = \min\{n, s\}.$$

Thus

$$\mathrm{rk}(C) = n = s.$$

It follows that $C$ is invertible, $\mathcal{M}$ has the same number of vertices and faces, and every face is incident to $d$ vertices. Moreover, Theorem 5.2.4 shows that for $U$ to have precisely two non-real eigenvalues, $CC^T$ must have precisely two eigenvalues, one of which is $d^2$. Using Lemma 5.1.2 and the fact that

$$\mathrm{tr}(CC^T) = d^2\,\mathrm{tr}(PQ) = nd,$$

we find the other eigenvalue:

$$\frac{(n-d)d}{n-1}.$$

Therefore,

$$CC^T = \frac{(n-d)d}{n-1} I + \frac{(d-1)d}{n-1} J.$$

This determines the eigenvalues $e^{\pm i\theta}$, as described in (i). For (ii), note that

$$C = BD^T,$$

so the rank of $C$ cannot exceed the rank of $B$ or the rank of $D$. In particular, if either $X$ or $X^*$ is bipartite, then $\mathrm{rk}(B) < n$ or $\mathrm{rk}(C) < n$, so $B$ cannot be invertible. □

For instance, the planar embedding $\mathcal{M}$ of $K_4$ has 4 vertices and 4 faces, where each vertex is incident to 3 faces, each face is incident to 3 vertices, and every two faces have 2 vertices in common. Thus the vertex-face walk relative to either orietation of $\mathcal{M}$ has exactly three eigenvalues.

Our initial goal is to find transition matrices whose $H$-weighted digraphs have as few weights as possible. Are there any among those with three eigenvalues? The answer is positive. In fact, all of them can be implemented as continuous quantum walks on oriented graphs.

**5.4.3 Theorem.** *Let $X$ be a connected $d$-regular graph on $n$ vertices. Let $U$ be the transition matrix of a vertex-face walk for a circular embedding of $X$. If $U$ has exactly three eigenvalues, then there is $\gamma \in \mathbb{R}$ such that*

$$U = \exp(\gamma(U^T - U)).$$

*Moreover, $U^T - U$ is a scalar munltiple of the skew-symmetric adjacency matrix of an oriented graph, which has*

*(i)* $n(n-1)$ *vertices,*

*(ii) valency*

$$\frac{d(n-d)(d-1)}{n-1},$$

*and*

*(iii) eigenvalues*

$$0, \quad \pm \arccos\left(\frac{2(n-d)}{d(n-1)} - 1\right).$$

*Proof.* By Theorem 5.4.2, the eigenprojections of $CC^T$ are

$$E_{d^2} = \frac{1}{n}J, \quad E_\mu = I - \frac{1}{n}J.$$

It follows from Lemma 5.3.1 that the Hamiltonian is an imaginary multiple of

$$\begin{aligned} \widehat{N}E_\mu\widehat{N}^T P - P\widehat{N}E_\mu\widehat{N} &= \widehat{N}\widehat{N}P - P\widehat{N}\widehat{N} \\ &= QP - PQ \\ &= \frac{1}{4}(U^T - U). \end{aligned}$$

Moreover, since both $X$ and $X^*$ are $d$-regular, Property (iii) of Lemma 5.1.2 shows that

$$(QP-PQ)_{(a,b),(u,v)} = \begin{cases} \dfrac{1}{d^2}, & \text{if } a \in f_{uv} \text{ and } u \notin f_{ab}, \\ -\dfrac{1}{d^2}, & \text{if } a \notin f_{uv} \text{ and } u \in f_{ab} \\ 0, & \text{otherwise.} \end{cases}$$

We compute the valency of the underlying digraph. Fix an arc $(u, v)$. For every positive entry of $(QP-PQ)e_{uv}$, we need an arc $(a, b)$ such that $a \in f_{uv}$ and $u \notin f_{ab}$. Due to the bijection between outgoing arcs of $a$ and faces using $a$, effectively we are counting pairs $(a, h)$ of vertex $a$ and face $h$, where $a$ is on $f_{uv}$, and $h$ is on $a$ but not on $u$. Note that such a pair must have $a \neq u$. On the other hand, for each $a \neq u$ on $f_{uv}$, there are $d$ faces on $a$, of which

$$\frac{(d-1)d}{n-1}$$

are also on $u$. Therefore, the number of positive entries in $(QP-PQ)e_{uv}$ is

$$(d-1)\left(d-\frac{(d-1)d}{n-1}\right) = \frac{d(n-d)(d-1)}{n-1}.$$

Finally, since $U\mathbf{1} = U^T\mathbf{1} = \mathbf{1}$, there are as many negative entries as positive entries in each column of $U^T - U$. The eigenvalues of the $H$-weighted digraph follow from Theorem 5.4.2. □

Of course, our quantum walk is based on more than just an incidence structure—not every vertex-face incidence matrix can be realized by a circular embedding. In addition to the obvious conditions for a symmetric 2-design to exist, we also need the following, at the very least.

(i) The parameter

$$\frac{(d-1)d}{n-1}$$

is a positive integer greater than one, since every edge is used by two faces.

(ii) The product $nd$ must be divisible by 4, due to Euler's formula

$$n - \frac{nd}{2} + n = 2 - 2g.$$

Two candidates for the vertex-face incidence structure are the trivial design, and the projective geometry design with parameters

$$\left(\frac{q^k-1}{q-1}, \frac{q^{k-1}-1}{q-1}, \frac{q^{k-2}-1}{q-1}\right).$$

We move on to the case where $U$ has exactly four eigenvalues, that is, 1, $-1$ and two complex numbers on the unit circle. We have the following characterization in terms of $C$.

**5.4.4 Theorem.** *Let $X$ be a connected $d$-regular graph on $n$ vertices. Let $U$ be the transition matrix of a vertex-face walk for a circular embedding of $X$. Let $C$ be the vertex-face incidence matrix. Then $U$ has exactly four eigenvalues if and only if $CC^T$ has exactly three eigenvalues, two of which are $d^2$ and 0.*

*Proof.* We prove one direction. Suppose $U$ has exactly four eigenvalues. By Theorem 5.2.3 we need either $\operatorname{rk}(C) < n$ or $\operatorname{rk}(C) < s$, so $C$ is not invertible. It follows that $CC^T$ has at least two eigenvalues: 0 and $d^2$. Moreover, for $U$ to have exactly two complex eigenvalues, there must be one more eigenvalue of $CC^T$ lying between 0 and $d^2$. □

## 5.5 Graph-Encoded Maps

Rotation systems are one way to describe orientable embeddings. In this section, we introduce another system, called graph-encoded maps, which encodes embeddings that could be orientable or non-orientable.

Let $\mathcal{M}$ be an embedding, where every face is bounded by a cycle. A *flag* is a triple $(u, e, f)$ of vertex $u$, edge $e$ and face $f$, where $u$ is incident to $e$, and $e$ is incident to $f$. Pictorially, a flag is a triangle in the barycentric division of a face. Figure 5.3 gives the planar embedding of $C_3$, for which every dot represents a flag.

For each flag $(u, e, f)$, let $u'$ be the other endpoint of $e$, let $e'$ be the other edge in $f$ that is incident to $u$, and let $f'$ be the other face that contains $e$. Define three functions

$$\begin{aligned}\tau_0 :&(u, e, f) \mapsto (u', e, f),\\ \tau_1 :&(u, e, f) \mapsto (u, e', f),\end{aligned}$$

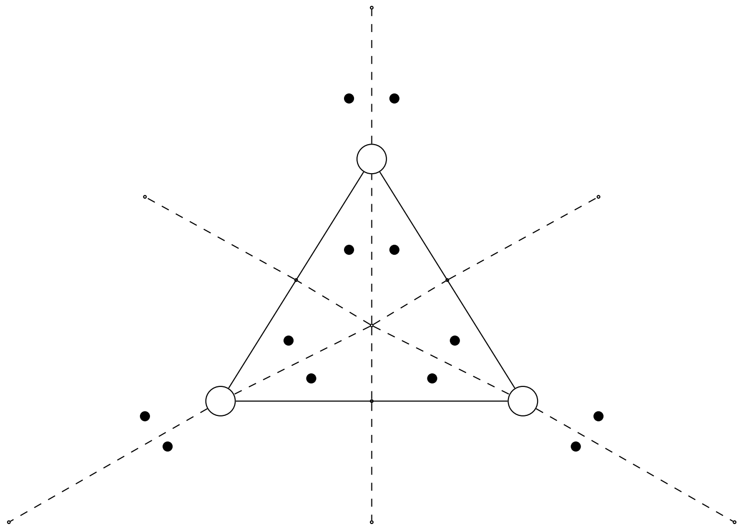


Figure 5.3: Planar embedding of $C_3$ and the flags

$$\tau_2 :(u, e, f) \mapsto (u, e, f').$$

We have the following observations.

(i) $\tau_0, \tau_1, \tau_2$ are fixed-point-free involutions.

(ii) $\tau_0\tau_2 = \tau_2\tau_0$, and $\tau_0\tau_2$ is fixed-point-free.

(iii) The group $\langle\tau_0, \tau_1, \tau_2\rangle$ acts transitively on the flags.

If we join two flags in Figure 5.3 by an edge whenever they are swapped by one of $\tau_0$, $\tau_1$ and $\tau_2$, then we obtain a cubic graph with a 3-edge-coloring, as shown in Figure 5.4.

In general, for an embedding $\mathcal{M}$, a *graph-encoded map*, or *gem*, is a cubic graph with a 3-edge coloring, where the vertices are the flags, and the 3-edge coloring is induced by the three involutions $\tau_0$, $\tau_1$ and $\tau_2$, as described above. The concept of gem was first introduced by Lins in [50], where he also proved the following characterization of orientability.

**5.5.1 Theorem.** *An embedding is orientable if and only if the gem is bipartite.* □

Note that an embedding $\mathcal{M}$ with $\ell$ edges has $4\ell$ flags. Thus, if $\mathcal{M}$ is orientable, then there are two components in the distance-2 graph of the

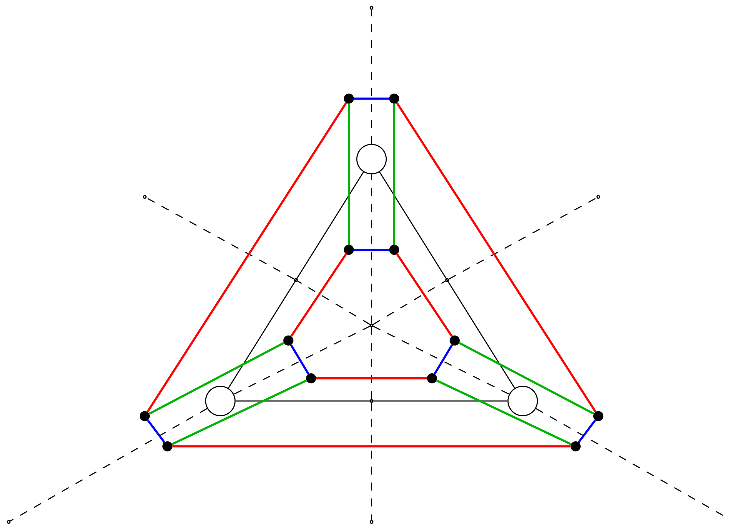


Figure 5.4: Planar embedding of $C_3$ and the gem

gem, each with $2\ell$ vertices. Let $Y$ be one such component. We claim that the vertex-face walk for $\mathcal{M}$ is equivalent to a two-reflection walk on $Y$. Let $\pi_1$ be the partition of the vertices $(u, e, f)$ of $Y$ based on their third coordinates $f$. It is not hard to see that the size of each cell in $\pi_1$ is the degree of some face. Similarly, let $\pi_2$ be the partition of $V(Y)$ based on their first coordinates $u$. Let $\widehat{M}$ and $\widehat{N}$ be the normalized characteristic matrices for $\pi_1$ and $\pi_2$, respectively. Then

$$(2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I)$$

is precisely the vertex-face walk for $\mathcal{M}$ relative to one consistent orientation of the faces.

One advantage of using gems is that our definition of vertex-face walks can be extended to non-orientable embeddings; we will discuss this at the end of this chapter.

## 5.6 Sparse Hamiltonians from Regular Embeddings

In this section, we show that for every prime power $n$, a regular embedding of $K_n$ yields a vertex-face walk with exactly three eigenvalues. This provides an infinite family of discrete quantum walks that can be implemented using continuous quantum walks on unweighed digraphs.

We start by introducing some basic concepts on rotation systems. For more background, see Gross and Tucker [38]. A *rotation system* is a set $\{\pi_u : u \in V(X)\}$ where each $\pi_u$ is a cyclic permutation on the neighbors of the vertex $u$. For any arc $(u_1, u_2)$, consider the walk

$$(u_1, u_2), (u_2, u_3), (u_3, u_4), \cdots, (u_{k-1}, u_k), \cdots$$

where

$$u_{j+1} = \pi_{u_j}(u_{j-1}).$$

Since the graph is finite, eventually this walk will meet an arc that is already taken. Moreover, the first arc that is used twice must be $(u_1, u_2)$, as the preimage $\pi_u^{-1}(v)$ is uniquely determined for each $u$. Therefore this walk is closed with no repeated arc. All closed walks arising in this way partition the arcs of $X$; they are precisely the facial walks, as we have seen. For each facial walk of length $k$, we associated it with a polygon with $k$ sides, labeled by the arcs in the same order as they appear in the walk. We then “glue” each two sides of these polygons labeled by the same edge. This results in an embedding of the graph onto an orientable surface.

An embedding $\mathcal{M}$ of a graph $X$ is *graph self-dual* if the dual graph $X^*$ is isomorphic to $X$. For the complete graph $K_n$, the dual graph is regular on $n$ vertices if and only if $\mathcal{M}$ is graph self-dual. If this embedding is circular, in addition to being graph self-dual, then the vertex-face incidence structure is the complement of a trivial design, that is, $C$ can be obtained from $J - I$ by permuting the rows and columns.

Using Euler’s formula, one can show that $K_n$ has a graph self-dual embedding only if $n \equiv 0, 1 \pmod 4$. The other direction requires clever constructions, and has been proved several times independently. For one of these treatments, see White [63].

**5.6.1 Theorem.** *The complete graph $K_n$ has a graph self-dual orientable embedding if and only if $n \equiv 0, 1 \pmod 4$.* □

However, not all graph self-dual embeddings of $K_n$ are circular. In fact, such constructions are only known for $K_n$ with $n$ a prime power, due to Biggs [13]. We describe his rotation systems in the following theorem.

**5.6.2 Theorem.** *Let $n = p^k$ for some prime $p$. Let $g$ be a primitive generator of the finite field $\mathbb{F}$ of order $n$. For each element $u$ in $\mathbb{F}$, define the cyclic permutation*

$$\pi_u := (v + g^0, v + g^1, \cdots, v + g^{n-2}).$$

*The rotation system $\{\pi_u : u \in V(K_n)\}$ gives a circular embedding of $K_n$.*

*Proof.* The complete graph $K_n$ can be viewed as as Cayley graph over $\mathbb{F}$. Clearly, $\pi_u$ is a permutation on the neighbors of $u$. Further, the facial walk containing arc $(v, v + g^0)$ visits vertices in the following order

$$v, v + g^0, v + g^0 - g^1, v + g^0 - g^1 + g^2, \cdots$$

Since

$$\sum_{j=0}^{m-1} (-g)^j = \frac{1 - (-g)^m}{1 + g}$$

is distinct for $m = 0, 1, \cdots, n - 2$, this facial walk has length $n - 1$ with no vertex repeated. Therefore the embedding is circular and graph self-dual. □

An embedding $\mathcal{M}$ is *regular* if the group generated by the three involutions $\langle \tau_0, \tau_1, \tau_2 \rangle$ acts regularly on the flags. Biggs showed that $K_n$ has a regular embedding if and only if $n$ is a prime power, and every regular embedding of $K_n$ must arise from the rotation system described above [13]. Using his construction, we find an infinite family of vertex-face walks whose transition matrices are also transition matrices of continuous quantum walks on oriented graphs.

**5.6.3 Theorem.** *Let $n$ be a prime power. Let $U$ be the transition matrix of the vertex-face walk for a regular embedding of $K_n$. Then there is $\gamma \in \mathbb{R}$ such that*

$$U = \exp(\gamma(U^T - U)).$$

*Moreover, $U^T - U$ is a scalar multiple of the skew-symmetric adjacency matrix of an oriented graph, which*

*(i) has $n(n-1)$ vertices,*

*(ii) is $(n-2)$-regular, and*

*(iii) has exactly three eigenvalues: $0$ and $\pm i\sqrt{n^2 - 2n}$.*

*Proof.* We have

$$CC^T = I + (n-2)J,$$

So the eigenvalues of $U$ are 1 and $e^{i\theta}$, where

$$\cos(\theta) = \frac{2}{(n-1)^2} - 1.$$

By Lemma 5.3.1 and Theorem 5.4.3, the Hamiltonian is

$$H = \frac{2i\theta}{\sin(\theta)}(QP - PQ) = \frac{2i\theta}{(n-1)^2\sin(\theta)}A(Z),$$

where $A(Z)$ is the skew-symmetric adjacency matrix of the digraph underlying $H$. The eigenvalues of $A(Z)$ then follows from the eigenvalues of $H$. □

Figure 5.5 shows the $H$-digraph of the planar embedding of $K_4$.

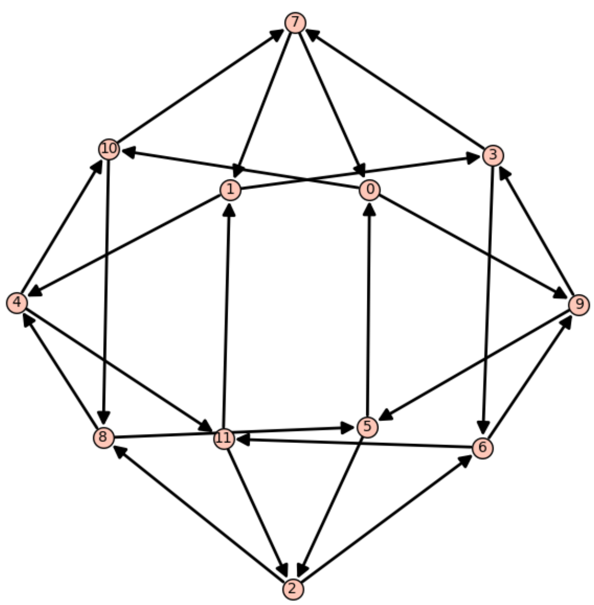



Figure 5.5: $H$-weighted digraph for the planar embedding of $K_4$

## 5.7 Covers

Before moving on to transition matrices with four eigenvalues, we spend a section understanding covers of embeddings. This provides a natural way to "lift" vertex-face walks.

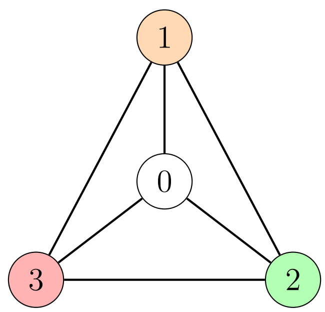



Figure 5.6: $K_4$

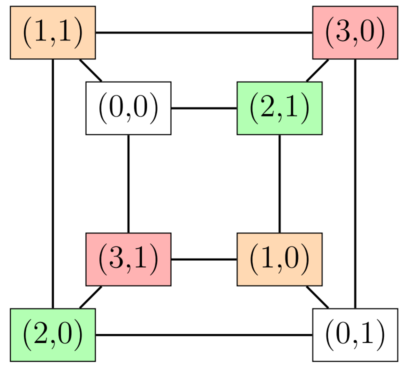



Figure 5.7: A double cover of $K_4$

An *arc-function of index* $r$ of $X$ is a map $\phi$ from the arcs of $X$ into $\mathrm{Sym}(r)$, such that $\phi(u,v) = \phi(v,u)^{-1}$. The *fiber* of a vertex $u$ is the set

$$\{(u,j) : j = 0, 1, \cdots, r-1\}.$$

If we replace each vertex of $X$ by its fiber, and join $(u,j)$ to $(v,k)$ whenever $\phi(u,v)(j) = k$, then we obtain a new graph $X^\phi$, called the *r-fold cover* of $X$. For example, we can let $\phi$ be the constant arc-function that sends every arc to $(1,2) \in \mathrm{Sym}(2)$. Then the double cover $K_4^\phi$ is isomorphic to the cube, as shown in Figure 5.7.

The above definition tells us how to construct a cover from a base graph. Alternatively, we say a graph $Y$ *covers* $X$ if there is a homomorphism $\psi$ from $Y$ to $X$, such that for any vertex $y$ of $Y$ and $x = \psi(y)$, the homomorphism $\psi$ restricted to $N_Y(y)$ is a bijection onto $N_X(x)$. The map $\psi$ is called a *covering map*. If $X$ is connected, then the preimages $\psi^{-1}(x)$ all have the same size; they are precisely the fibers of $X$.

Given an orientable embedding $\mathcal{M}_X$ of $X$, and a covering map $\psi$ from a connected graph $Y$ to $X$, we define an orientable embedding $\mathcal{M}_Y$ of $Y$ by specifying its facial walks; such an embedding will be called the *embedding induced by* $(\mathcal{M}_X, \psi)$, or the *embedding induced by* $(\mathcal{M}_X, \phi)$ if $\phi$ is the corresponding arc-function. Let $W$ be a facial walk of $\mathcal{M}_X$ starting at vertex $u$. Clearly, the preimage $\psi^{-1}(W)$ consists of walks starting and ending in the fiber $\psi^{-1}(u)$, and each arc of $Y$ appears in at most one of these walks. Then, the facial walks of $\mathcal{M}_Y$ are exactly the closed walks in the preimages of the facial walks of $\mathcal{M}_X$. In the previous example, the planar embedding of $K_4$ gives rise to an embedding of the cube on the torus, with 4 faces, each of length 6.

We will focus on a special type of cover, known as the voltage graphs. A *voltage graph* of $X$ is an $r$-fold cover $Y = X^{\phi}$, where the image of the arc-function $\phi$ is a subgroup $\Gamma \leq \mathrm{Sym}(r)$ of order $r$, and

$$V(Y) = V(X) \times \Gamma, \quad E(Y) = E(X) \times \Gamma.$$

Voltage graphs correspond to normal covers [40], and have been extensively studied. We only state one property that voltage graphs satisfy; for more background, see Gross and Tucker [38].

**5.7.1 Theorem.** *Let $X$ be a graph. Let $Z$ be a $k$-cycle in $X$. Let $Y = X^{\phi}$ be a voltage graph of order $r$. If $\phi(Z)$ has order $\ell$, then the components of $F(Z)$ consists of $r/\ell$ cycles, each of length $k\ell$.* □

The next result shows that the transition matrix of $X$ is a block sum of the transition matrix of its voltage graph. To prove it, we need the concept of equitable partition, due to Godsil [25, Ch 12]. Let $A$ be a matrix over $\mathbb{C}$. Let $\sigma$ and $\rho$ be the partition of the columns and rows of $A$, and let $K$ and $L$ be their respective characteristic matrices. The pair $(\rho, \sigma)$ is *column equitable* if $\mathrm{col}(AK) \subseteq \mathrm{col}(L)$, *row equitable* if $\mathrm{col}(A^*L) \subseteq \mathrm{col}(K)$, and *equitable* if it is both column and row equitable.

**5.7.2 Theorem.** *Let $X$ be a graph. Let $Y = X^{\phi}$ be a voltage graph of $X$. Let $\rho$ be the partition of the arcs of $Y$, where each class is the preimage of some arc of $X$. Let $\widehat{L}$ be its normalized incidence matrix of $\rho$. If $U_X$ and $U_Y$ are the transition matrices for the corresponding embeddings of $X$ and $Y$, then*

$$U_X = \widehat{L}^T U_Y \widehat{L}.$$

*Proof.* Write $U_Y$ as

$$U_Y = (2\widehat{M_Y}\widehat{M_Y^T} - I)(2\widehat{N}_Y\widehat{N}_Y^T - I).$$

Let $\sigma$ be the partition of the vertices of $Y$ into fibers, with normalized incidence matrix $\widehat{K}$. It is not hard to verify that

$$\widehat{N}_Y\widehat{K} = \widehat{L}\widehat{N}_X$$

and

$$\widehat{N}_Y^T\widehat{L} = \widehat{K}\widehat{N}_X^T.$$

Thus $(\rho, \sigma)$ is an equitable partition of $\widehat{N}_Y$ [25, Ch 12]. It follows that

$$\widehat{N}_Y \widehat{K} \widehat{K}^T = \widehat{L} \widehat{L}^T \widehat{N}_Y. \tag{5.7.1}$$

Since

$$\widehat{N}_X = \widehat{L}^T \widehat{N}_Y \widehat{K},$$

the projection onto its column space can be written as

$$\begin{aligned} \widehat{N}_X \widehat{N}_X^T &= \widehat{L}^T (\widehat{N}_Y \widehat{K} \widehat{K}^T) \widehat{N}_Y^T \widehat{L} \\ &= \widehat{S}^T (\widehat{L} \widehat{L}^T \widehat{N}_Y) \widehat{N}_Y^T \widehat{L} \\ &= \widehat{L}^T \widehat{N}_Y \widehat{N}_Y^T \widehat{L}. \end{aligned}$$

Applying a similar argument to the preimages of facial walks, we can show that

$$\widehat{M}_X \widehat{M}_X^T = \widehat{L}^T \widehat{M}_Y \widehat{M}_Y^T \widehat{L}.$$

Thus,

$$U_X = \widehat{L}^T (2 \widehat{M}_Y \widehat{M}_Y^T - I) \widehat{L} \widehat{L}^T (2 \widehat{N}_Y \widehat{N}_Y^T - I) \widehat{L}. \tag{5.7.2}$$

Finally, from Equation (5.7.1) we see that

$$\widehat{L} \widehat{L}^T \widehat{N}_Y \widehat{N}_Y^T = \widehat{N}_Y \widehat{K} \widehat{K}^T \widehat{N}_Y^T$$

is a symmetric matrix, and so $\widehat{S} \widehat{S}^T$ commutes with $\widehat{N}_Y \widehat{N}_Y^T$. Therefore, Equation (5.7.2) reduces to

$$U_X = \widehat{L}^T U_Y \widehat{L}.$$

□

## 5.8 Sparse Hamiltonians from Covers

If $U$ has exactly four eigenvalues, then they must be $1$, $-1$ and $e^{\pm i\theta}$. Thus

$$H = \pi F_{-1} + \theta (F_+ - F_-),$$

where $F_\pm$ is the projection onto the $e^{\pm i\theta}$-eigenspace. As a consequence, the $H$-weighted digraph splits into two weighted digraphs, whose Hermitian adjacency matrices are orthogonal.

In this section, we construct an infinite family of circular embeddings for which $U$ has four eigenvalues, and the $H$-weighted digraph has only distinct weights on the arcs. These are embeddings of $K_2 \times K_n$ that arise from regular embeddings of $K_n$. The first example in the infinite family is the embedding of the cube, viewed as the double cover $K_2 \times K_4$ in Figure 5.7, with facial walks

$$\begin{aligned} f_0 &= \{(0,0),(1,1),(2,0),(0,1),(1,0),(2,1)\}; \\ f_1 &= \{(3,0),(2,1),(1,0),(3,1),(2,0),(1,1)\}; \\ f_2 &= \{(2,0),(3,1),(0,0),(2,1),(3,0),(0,1)\}; \\ f_3 &= \{(0,0),(3,1),(1,0),(0,1),(3,0),(1,1)\}. \end{aligned}$$

In general, the facial walks of our embedding of $K_2 \times K_n$ are preimages of the facial walks of a regular embedding of $K_n$.

**5.8.1 Lemma.** *Let $n$ be a power of 2. Let $\mathcal{M}$ be a regular embedding of $K_n$. Let $\phi$ be the 2-fold arc-function that sends every arc of $X$ to $(1,2) \in \mathrm{Sym}(2)$. Let $\mathcal{M}'$ be the embedding of $K_2 \times K_n$ induced by $(M', \phi)$. Let $M$ and $M'$ be the arc-face incidence matrices for $\mathcal{M}$ and $\mathcal{M}'$. Let $N$ and $N'$ be the arc-tail incidence matrices for $\mathcal{M}$ and $\mathcal{M}'$. Let $\rho$ be the partition of the arcs of $K_2 \times K_n$, where each class is the preimage of some arcs of $K_n$. Let $L$ be the incidence matrix of $\rho$. We have*

*(i)* $N' = 2LN$;

*(ii)* $M' = LM$.

*Proof.* (i) is immediate. For (ii), note that every facial cycle $Z$ in $K_n$ has odd length $n-1$, so $\phi(Z) = (1,2)$ and the preimage of $Z$ is a facial cycle of length $2(n-1)$. It follows that a facial walk in $\mathcal{M}'$ contains $((u,1),(v,2))$ if and only if it contains $((u,2),(v,1))$. □

**5.8.2 Corollary.** *Let $n$ be a power of 2. Let $\mathcal{M}$ be a regular embedding of $K_n$. Let $\phi$ be the 2-fold arc-function that sends every arc of $X$ to the element $(1,2) \in \mathrm{Sym}(2)$. Let $\mathcal{M}'$ be the embedding of $K_2 \times K_n$ induced by $(M', \phi)$. Let $C$ and $C'$ be the vertex-face incidence matrices for $\mathcal{M}$ and $\mathcal{M}'$. We have*

*(i)* $(C')^T C' = 2C^T C$;

*(ii)* $C'(C')^T = \dfrac{1}{n-1} CC^T \otimes J_2$.

*Proof.* The first part follows from the previous Lemma 5.8.1. To see the second part, note that for any vertex $u$ of $K_n$, the vertex $(u, 1)$ appears in a face $f$ of $K_2 \times K_n$ if and only if $(u, 2)$ appears in $f$. Since

$$CC^T = I_n + (n-2)J_n,$$

two vertices of $Y$ in the same fiber lie in exactly $n-1$ faces, and two vertices from different fibers lie in exactly $n-2$ faces. Applying Property (iv) in Lemma 5.1.2 yields the identity. □

**5.8.3 Corollary.** *Let $n$ be a power of 2. Let $\mathcal{M}$ be a regular embedding of $K_n$. Let $\phi$ be the 2-fold arc-function that sends every arc of $X$ to the element $(1,2) \in \mathrm{Sym}(2)$. Let $\mathcal{M}'$ be the embedding of $K_2 \times K_n$ induced by $(M', \phi)$. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$. Let $U'$ be the transition matrix of the vertex-face walk for $\mathcal{M}'$. We have the following.*

*(i) The complex eigenvalues of $U'$ are the same as the complex eigenvalues of $U$, with the same multiplicity.*

*(ii) $-1$ is an eigenvalue of $U'$. Moreover, the eigenspace is spanned by the vectors $y_u$ over all vertices $u$ of $K_n$, where $y_u$ is $1$ on the outgoing arcs of $(u, 0)$, and $-1$ on the outgoing arcs of $(u, 1)$, and $0$ elsewhere.*

*Proof.* The first part follows from Corollary 5.8.2 (i). Let $M'$ and $N'$ be the arc-face incidence matrix and the arc-tail incidence matrix of $\mathcal{M}'$. Let $P'$ and $Q'$ be the orthogonal projections onto $\mathrm{col}(M')$ and $\mathrm{col}(N')$, respectively. From Corollary 5.8.2 (ii) we also see that

$$\mathrm{col}(P') \cap \ker(Q') = \{0\}.$$

Since each $y_u$ is constant on the outgoing arcs of each vertex of $K_2 \times K_n$, and $y_u$ sum to zero over each face of $\mathcal{M}'$, the set

$$\{y_u : u \in V(X)\}$$

forms an orthogonal basis of

$$\ker(P') \cap \mathrm{col}(Q').$$

This proves the second part. □

Our main result of this section is that the $H$-weighted digraph of the vertex-face walk for $\mathcal{M}'$ splits into two unweighted digraphs, whose Hermitian adjacency matrices are orthogonal.

**5.8.4 Theorem.** *Let $n$ be a power of 2. Let $\mathcal{M}$ be a regular embedding of $K_n$. Let $\phi$ be the 2-fold arc-function that sends every arc of $X$ to the element $(1,2) \in \mathrm{Sym}(2)$. Let $\mathcal{M}'$ be the embedding of $K_2 \times K_n$ induced by $(M', \phi)$. Let $U$ be the transition matrix of the vertex-face walk for $\mathcal{M}$. Let $U'$ be the transition matrix of the vertex-face walk for $\mathcal{M}'$. There is a real $\beta$ and an imaginary $\eta$ such that*

$$U' = \exp(\beta H_1 + \eta H_2),$$

*where*

$$H_1 = J_n \otimes \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \otimes J_{n-1},$$

*and*

$$H_2 = (U')^T - U' = (U^T - U) \otimes J_2.$$

*Moreover, $H_1 H_2 = 0$.*

*Proof.* Let $H$ be the Hamiltonian of $U'$. We have for some complex numbers $e^{\pm i\theta}$ that

$$H = \pi F_{-1} + \theta(F_+ - F_-).$$

By Corollary 5.8.3 (ii), the eigenprojection $F_{-1}$ is a real multiple of $H_1$.

Let $M$ and $N$ be the arc-face incidence matrix and the arc-tail incidence matrix for $\mathcal{M}$. Let $P$ and $Q$ denote the orthogonal projections on $\mathrm{col}(M)$ and $\mathrm{col}(N)$, respectively. From Lemma 5.3.1, Theorem 5.4.3 and Lemma 5.8.1, we see that $F_+ - F_-$ is an imaginary multiple of

$$Q\widehat{L}W\widehat{L}^T - \widehat{L}W\widehat{L}^T Q,$$

where

$$W = P - \frac{1}{n(n-1)} J_{n(n-1)}.$$

Applying Lemma 5.8.1 again yields the expression for $H_2$. □

If follows that $(U')^2$ is the transition matrix of a continuous quantum walk on an oriented graph.

**5.8.5 Theorem.** *Let $n$ be a power of 2. Let $\mathcal{M}$ be a regular embedding of $K_n$. Let $\phi$ be the 2-fold arc-function that sends every arc of $X$ to the element $(1,2) \in \mathrm{Sym}(2)$. Let $\mathcal{M}'$ be the embedding of $K_2 \times K_n$ induced by $(M', \phi)$. Let $U'$ be the transition matrix of the vertex-face walk for $\mathcal{M}'$. Then there is $\gamma \in \mathbb{R}$ such that*

$$(U')^2 = \exp(\gamma((U')^T - U')).$$

*Moreover, $(U')^T - U'$ is a scalar multiple of the skew-symmetric adjacency matrix of an oriented graph, which*

*(i) has $2n(n-1)$ vertices,*

*(ii) is $(n-2)$-regular, and*

*(iii) has exactly three eigenvalues: 0 and $\pm 2i\sqrt{n^2 - 2n}$.* □

## 5.9 Sedentary Walks

One counterintuitive phenomenon in quantum walks is that the walker may be reluctant to leave its initial state. This was first observed in continuous quantum walks on $K_n$: for any time $t$, the mixing matrix

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

converges to $I$ as $n$ goes to infinity. In [30], Godsil investigated quantum walks on complete graphs, some cones and some strongly regular graphs that enjoy the same property. Following his paper, we say a sequence of discrete quantum walks, determined by transition matrices $\{U_1, U_2, \cdots\}$, is *sedentary* if for any step $K$, the mixing matrices $U_n^k \circ \overline{U_n^k}$ converges to $I$ as $n$ goes to infinity. Both families studied in earlier sections exhibit this phenomenon.

**5.9.1 Theorem.** *For each prime power $n$, let $U_n$ be the vertex-face walk for a regular embedding of $K_n$. The quantum walks determined by*

$$\{U_n : n \text{ is a prime power}\}$$

*form a sedentary family.*

*Proof.* Fix $n$ and $k$. We compute the diagonal entries of the mixing matrix $U^k \circ U^k$. Recall that the non-real eigenvalues of $U_n$ are $e^{\pm i\theta}$, where

$$\cos(\theta) = \frac{2}{(n-1)^2} - 1.$$

Let $F_\pm$ be the orthogonal projection onto the $e^{\pm i\theta}$-eigenspace of $U$. Corollary 5.2.5 says that that $F_\pm$ is a linear combination of the four matrices:

$$W, \quad PW, \quad WP, \quad PWP, \tag{5.9.1}$$

where

$$W = \widehat{N}\left(I - \frac{1}{n}J\right)\widehat{N}^T = Q - \frac{1}{n}J.$$

Using Lemma 5.1.2 it is not hard to see that all four matrices in Equation 5.9.1 have constant diagonal. Thus $F_+$ and $F_-$ have constant diagonal. As as linear combination of

$$F_+, \quad F_-, \quad F_1 = I - F_+ - F_-,$$

the power $U^k$ also has constant diagonal. On the other hand, the trace of $U^k$ can be computed its spectrum. By Theorem 5.2.4, both $e^{i\theta}$ and $e^{-i\theta}$ have multiplicity $n-1$, so 1 has multiplicity $(n-2)(n-1)$. It follows that

$$\operatorname{tr}(U^k) = (n-2)(n-1) + 2\cos(k\theta)(n-1).$$

Hence, each diagonal entry if $U_n^k \circ U_n^k$ equals

$$\left(1 - \frac{2 - 2\cos(k\theta)}{n}\right)^2,$$

which converges to 1 as $n$ tends to infinity. □

**5.9.2 Theorem.** *For each $n$ that is a power of 2, let $\mathcal{M}$ be a regular embedding of $K_n$, and let $\phi$ be the 2-fold arc-function that sends every arc of $K_n$ to $(1,2) \in \mathrm{Sym}(2)$. Let $U'_n$ be the transition matrix of the embedding of $K_2 \times K_n$ induced by $(\mathcal{M}, \phi)$. The quantum walks determined by*

$$\{U'_n : n \text{ is a power of } 2\}$$

*form a sedentary family.*

*Proof.* Fix $n$ and $k$. The eigenvalues of $U^k$ are 1, $-1$ and $e^{\pm ik\theta}$, where

$$\cos(\theta) = \frac{2}{(n-1)^2} - 1.$$

Again, one can check that the projections $F_1$, $F_{-1}$ and $F_{\pm}$ onto the eigenspaces have constant diagonal. Moreover, by Theorem 5.2.3 and Theorem 5.2.4,

$$\operatorname{rk}(F_1) = 2(n-1)^2 - n, \quad \operatorname{rk}(F_{-1}) = n, \quad \operatorname{rk}(F_{\pm}) = n-1.$$

Therefore

$$\operatorname{tr}(U_n^k) = 2(n-1)^2 - n + (-1)^k n + 2\cos(k\theta)(n-1).$$

It follows that each diagonal entry of $U_n^k \circ U_n^k$ is

$$\left(1 - \frac{2-2\cos(k\theta)}{2n} + \frac{(-1)^2 - 1}{2(n-1)}\right)^2,$$

which converges to 1 as $n$ goes to infinity. □

## 5.10 Open Problems

At the end of this chapter, we mention some open problems related to the vertex-face walks.

Theorem 5.4.3 characterizes all vertex-face incidence structures for which the transition matrix has precisely three eigenvalues. So far, the only known examples are regular embeddings of complete graphs. It remains open whether a non-complete graph has an embedding that satisfies Theorem 5.4.3. One approach we can take is to check if there exist other $H$-digraphs with parameters given by Theorem 5.4.3.

(i) Characterize digraphs on $n(n-1)$ vertices, with valency

$$\frac{d(n-d)(d-1)}{n-1},$$

and eigenvalues

$$0, \quad \pm \arccos\left(\frac{2(n-d)}{d(n-1)} - 1\right).$$

Another more direct approach is to investigate whether a symmetric 2-design can be realized by the vertex-face incidence structure of an existing embedding. More generally, we would like to answer the following.

(ii) Given an incidence structure with points $V$ and blocks $F$, can we construct an orientable embedding with $V$ as vertices and $F$ as faces?

Our original definition of a vertex-face walk requires the embedding to be orientable, since the arc-face partition is based on a consistent orientation of the faces. However, the discussion at the end of Section 5.5 provides a way to generalize vertex-face walks to non-orientable embeddings. Let $Y$ be the gem of an embedding $\mathcal{M}$, where every face is bounded by a cycle. Let $\pi_1$ be coarsest partition of the flags, such that in each cell, all flags share an face, while no two flags share an edge. Similarly, let $\pi_2$ be the coarsest partition of the flags, such that in each cell, all flags share a vertex, while no two flags share an edge. Let $\widehat{M}$ and $\widehat{N}$ be the normalized characteristic matrices for $\pi_1$ and $\pi_2$, respectively. Then

$$U = (2\widehat{M}\widehat{M}^T - I)(2\widehat{N}\widehat{N}^T - I)$$

defines a quantum walk on $Y$, which is reducible if and only if $\mathcal{M}$ is orientable. In other words, each arc $(u, v)$ in the underlying graph $X$ is paired with two flags $(u, e, f)$ and $(u, e, f')$, and the probability that the walker is on the arc $(u, v)$ can be computed by summing the probabilities of her being on $(u, e, f)$ and $(u, e, f')$. There are many questions we may ask about this new definition of vertex-face walks; below are two examples.

(iii) How much can the limiting distribution of a vertex-face walk for an orientable embedding differ from that of a vertex-face walk for a non-orientable embedding?

(iv) Can we characterize non-orientable embeddings for which the $H$-weighted digraphs are sparse with few weights on the arcs?

Finally, our vertex-face model can be viewed as a generalization of the walk used by Ambainis et al in [6], for the spatial search on a 2-dimensional lattice. While their walk does not satisfy the locality condition, the travel distance for the quantum walker during one step is at most 2, which is a constant. By comparison, simply applying the Grover's search on the lattice requires the walker to travel across the entire database. Therefore, the moving cost is in some sense negligible.

We would like to know whether the vertex-face walk can be used to design other quantum algorithms. For spatial search on a regular graph $X$, let $u$ be the marked vertex and

$$V_u := (I - 2E_{uu}) \otimes I$$

the oracle operator. Since each step of a vertex-face walk is equivalent to two steps of the arc-reversal walk, we define the perturbed vertex-face walk to be

$$(2\widehat{M}\widehat{M}^T - I)V_u(2\widehat{N}\widehat{N}^T - I)V_u;$$

this is in the same form as the search operator in [6]. Compared to the arc-reversal search [5], the vertex-face search seems to have a higher success probability, as indicated by our numerical experiments. Of course, one needs to take into consideration the maximum distance of two vertices in a face, since a high moving cost may offset the speedup in the algorithm.

(v) Can we design other fast algorithms based on the vertex-face walks?

# Chapter 6

# Walking on Unitary Covers

When a particular model does not exhibit the desired property, our quantum walker seeks alternatives by changing the coins, the shunt-decompositions, or even the operator itself. One thing she has not tried, though, is to enlarge the state space she lives in.

In this chapter, we introduce quantum walks on unitary covers of digraphs; they can be seen as quantum walks on the base digraphs with enlarged state spaces. Our model generalizes the shunt-decomposition walks [2], as well as the Möbius quantum walks [53]. In the Möbius walk, the walker can rotate around the axis of movement while walking on the cycle, and the extra rotation space allows uniform average vertex mixing to occur with optimized mixing time [53].

We start by extending the definition of covers. For a digraph $X$, an $r$-fold unitary arc-function is a map $\phi$ from the arcs of $X$ to the unitary group of degree $r$. If the image of $\phi$ consists of only permutations, then $X^{\phi}$ is the usual cover we have seen in Section 5.7. Next, given a shunt-decomposition of $X$, we define what it means for $\phi$ to be "compatible with" the shunt-decomposition; such a unitary arc-function is called a shunt-function. Finally, for a digraph $X$ with shunt-function $\phi$, we construct a quantum walk on $X^{\phi}$, and study the spectral decomposition of its transition matrix. Numerical experiments show that such a walk allows uniform average vertex mixing to occur on $X$, even if it is impossible on the usual shunt-decomposition walk.

## 6.1 Unitary Covers

We have seen how covers give rise to interesting walks in Chapter 5. There are two parts in the definition of a cover that we can generalize: the underlying graph, and the arc-function.

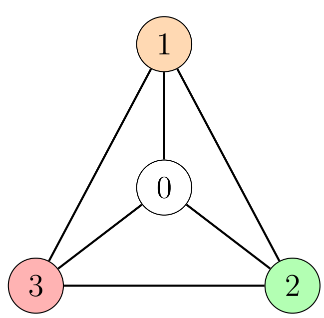
Let $X$ be a connected digraph. A *unitary arc-function of index* $r$ of $X$ is a map $\phi$ from the arcs of $X$ to $U(r)$, the unitary group of degree $r$, such that $\phi(u,v) = \phi(v,u)^{-1}$. Let $A(X)^{\phi}$ be the matrix obtained from $A(X)$ by replacing $A_{uv}$ with $\phi(u,v)$ if $(u,v)$ is an arc of $X$, and with an $r \times r$ block of zeros otherwise. The weighted digraph $X^{\phi}$ underlying $A(X)^{\phi}$ is called a *unitary $r$-fold cover*.

When the image of $\phi$ consists of only permutation matrices, we omit the word "unitary" and call $\phi$ an $r$-fold cover. If in addition $X$ is undirected, then we are back to the special case in Section 5.7. Recall that $X^{\phi}$ can be built as follows: replace each vertex $u$ of $X$ by its fiber:

$$\{(u,j) : i = 0, 1, \cdots, r-1\},$$

and join $(u,j)$ to $(v,k)$ whenever $\phi(u,v)(j) = k$. Alternatively, a digraph $Y$ covers $X$ if there is a homomorphism $\psi$ from $Y$ to $X$, such that for any vertex $y$ of $Y$ and $x = \psi(y)$, the homomorphism restricted to the outgoing arcs of $y$ in $Y$ is a bijection onto the outgoing arcs of $x$ in $X$.

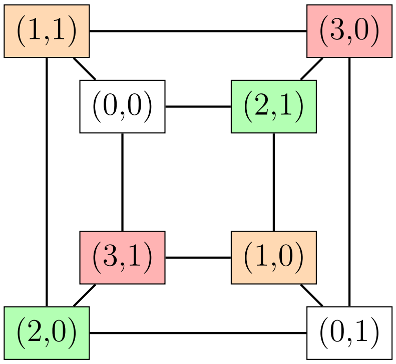
As shown in Figure 6.1 and Figure 6.2, the hypercube $Q_3$ is a double cover of the complete graph $K_4$, with covering map $\psi$ given by the vertex coloring. The arc-function $\phi$ sends every arc of $K_4$ to $(1,2) \in \mathrm{Sym}(2)$. We attach their adjacency matrices to illustrate the construction from $\phi$.




$$A(K_4) = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}$$

Figure 6.1: $K_4$ and its adjacency matrix

Most discussion of covers focuses on voltage graphs, see for example [38]. The *orthogonal covers*, for which the image of $\phi$ consists of only orthogonal




$$A(Q_3) = \left(\begin{array}{cc|cc|cc|cc} 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 1 & 0 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 \\ \hline 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \end{array}\right)$$

Figure 6.2: $Q_3$ and its adjacency matrix

matrices, have also been studied in [24]. In this chapter, we will consider unitary covers that respect shunt-decompositions, for they may preserve nice properties that the underlying digraphs admit.

## 6.2 Shunt-Functions

The aim of this section is to lift a shunt-decomposition walk on $X$ to a walk on its cover $X^\phi$. Our construction generalizes the shunt-decomposition model due to Aharonov et al [2], as well as the Möbius walk defined by Moradi and Annabestani [53].

Let $X$ be a $d$-regular digraph on $n$ vertices, with shunt-decomposition

$$A(X) = P_1 + \cdots + P_d.$$

We are interested in unitary arc-functions $\phi$ that are "compatible with" the shunt-decomposition, that is,

(i) for every arc $(u, v)$, the value $\phi(u, v)$ depends only on the shunt $(u, v)$ belongs to;

(ii) whenever $P_j$ and $P_j^T$ both appear as shunts, we have

$$\phi(P_j)^{-1} = \phi(P_j^T).$$

A unitary arc-function $\phi$ satisfying (i) and (ii) is called a *shunt-function*.

Given a shunt-function $\phi$, we define a quantum walk on $X^\phi$ as follows. Pick a $d \times d$ unitary coin $C$. The shift matrix $S$ is a $dnr \times dnr$ block diagonal matrix:

$$S = \begin{pmatrix} P_1 \otimes \phi(P_1) & & & \\ & P_2 \otimes \phi(P_2) & & \\ & & \ddots & \\ & & & P_d \otimes \phi(P_d) \end{pmatrix},$$

and the coin matrix is a $dnr \times dnr$ unitary matrix of the form

$$C \otimes I_n \otimes I_r.$$

Our new quantum walk on $X^\phi$, called the *shunt-function walk*, is then determined by the transition matrix

$$U := S(C \otimes I_n \otimes I_r).$$

We explain the connection between this walk and the ones in [2] and [53]. If $r = 1$ and $\phi$ is the identity map, then $X^\phi = X$ and the shift matrix is simply

$$S = \begin{pmatrix} P_1 & & & \\ & P_2 & & \\ & & \ddots & \\ & & & P_d \end{pmatrix}.$$

Thus $U$ coincides with the transition matrix of a shunt-decomposition walk on $X$. On the other hand, if $X$ is the $n$-cycle $C_n$, there is a shunt-decomposition

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

where $P$ is cyclic of order $n$. Suppose in addition that

$$\phi(P) = \begin{pmatrix} \cos\left(\frac{\theta}{2}\right) & i\sin\left(\frac{\theta}{2}\right) \\ i\sin\left(\frac{\theta}{2}\right) & \cos\left(\frac{\theta}{2}\right) \end{pmatrix}$$

and

$$\phi(P^{-1}) = \begin{pmatrix} \cos\left(-\frac{\theta}{2}\right) & i\sin\left(-\frac{\theta}{2}\right) \\ i\sin\left(-\frac{\theta}{2}\right) & \cos\left(-\frac{\theta}{2}\right) \end{pmatrix},$$

then our walk is precisely the Möbius walk defined in [53].

## 6.3 Spectral Decomposition

To simplify our analysis, we assume all shunts commute, and

$$\phi(P_j)\phi(P_k) = \phi(P_k)\phi(P_j).$$

The following lemma shows how to obtain the spectral decomposition of a shunt-function walk.

**6.3.1 Lemma.** *Let $X$ be a $d$-regular graph on $n$ vertices with shunt-decomposition*

$$A(X) = P_1 + \cdots + P_d.$$

*Let $\phi$ be a shunt-function of index $r$. Let*

$$U = S(C \otimes I_n \otimes I_r)$$

*be the transition matrix of a shunt-function walk on $X^\phi$. Let $y$ be a common eigenvector of the shunts, with*

$$P_j y = \lambda_j y.$$

*Let $z$ be a common eigenvector of $\phi(P_1), \phi(P_2), \cdots, \phi(P_d)$, with*

$$\phi(P_j)z = \mu_j z.$$

*Let $x$ be a vector of length $d$. Then $x \otimes y \otimes z$ is an eigenvector of $U$ for the eigenvalue $\alpha$ if and only if $x$ is an eigenvector of*

$$\begin{pmatrix} \lambda_1\mu_1 & & \\ & \ddots & \\ & & \lambda_d\mu_d \end{pmatrix} C$$

*for the eigenvalue $\alpha$.*

*Proof.* Rewrite

$$S = \sum_j E_{jj} \otimes P_j \otimes \phi(P_j).$$

Then

$$U = \sum_j E_{jj}C \otimes P_j \otimes \phi(P_j).$$

Let

$$D := \begin{pmatrix} \lambda_1\mu_1 & & \\ & \ddots & \\ & & \lambda_d\mu_d \end{pmatrix}.$$

We have

$$\begin{aligned} U(x \otimes y \otimes z) &= \sum_j E_{jj} C x \otimes P_j y \otimes \phi(P_j) z \\ &= \left( \sum_j \lambda_j \mu_j E_{jj} \right) C x \otimes y \otimes z \\ &= DCx \otimes y \otimes z. \end{aligned}$$

Thus $x \otimes y \otimes z$ is an eigenvector of $U$ for the eigenvalue $\alpha$ if and only if $x$ is an eigenvector of $DC$ for the eigenvalue $\alpha$. □

Using an argument similar to the proof of Theorem 3.6 in [2], we see that simple eigenvalues of $U$ guarantees uniform average vertex mixing.

**6.3.2 Lemma.** *Let $X$ be a Cayley digraph over an abelian group, with shunt-decomposition*

$$A(X) = P_1 + \cdots + P_d.$$

*Let $\phi$ be a shunt-function of index $r$, such that for all $j$ and $k$, we have $\phi(P_j) = \phi(P_k)$. Let*

$$U = S(C \otimes I_n \otimes I_r)$$

*be the transition matrix of a shunt-function walk on $X^\phi$. If $U$ has simple eigenvalues, then $U$ admits uniform average vertex mixing.* □

## 6.4 Open Problems

The shunt-function walks have not been studied in depth yet. Here are some problems we would like to work on.

The Möbius quantum walks allow uniform average vertex mixing to occur on all cycles [53]. In comparison, the usual shunt-decomposition walk with the same coin does not have uniform average vertex mixing, on any even cycle [2]. We wish to know if similar improvements can be made for other digraphs. Numerical experiments indicate that this is possible for many Cayley digraphs over abelian groups.

(i) Let $X$ be a Cayley digraph over an abelian group. Let

$$A = P_1 + \cdots + P_d$$

be the shunt-decomposition induced by the connection set. Let $C$ be a $d \times d$ unitary coin. Can we find a shunt-function $\phi$ for which $X^\phi$ admits uniform average vertex mixing?

On the other hand, some properties of a shunt-decomposition walk on $X$ may be preserved by a shunt-function $\phi$ of $X$. This leads to a different direction in comparing models of discrete quantum walks.

(ii) What is the relation between the shunt-decomposition walk on $X$ and a shunt-function walk on $X^\phi$?

# Chapter 7

# Appendix

## 7.1 Graph Theory

A *graph* is an ordered pair $(V, E)$ of *vertex set* $V$ and *edge set* $E$, where $E$ is a subset of $V \times V$. A *digraph* is an ordered pair $(V, \mathcal{A})$ of *vertex set* $V$ and *arc set* $\mathcal{A}$, where $\mathcal{A}$ consists of ordered pairs of vertices, called *arcs*. Given an arc $(u, v)$, its *tail* is $u$, and its *head* is $v$. An *oriented graph* is a digraph $(V, \mathcal{A})$ where, for any vertices $u$ and $v$, at most one of $(u, v)$ and $(v, u)$ is in $\mathcal{A}$.

In this thesis, we may treat a graph $(V, E)$ as a digraph $(V, \mathcal{A})$, where $\mathcal{A}$ contains arcs $(u, v)$ and $(v, u)$ whenever $\{u, v\}$ is in $E$.

Let $u$ be a vertex of a digraph $X$. The *out-neighbors* of $u$ are vertices $v$ such that $(u, v)$ is an arc, and the *out-degree* of $u$ is the number of its out-neighbors. $X$ is *$d$-out-regular* if all vertices have out-degree $d$. The *in-neighbors* of $u$ are vertices $v$ such that $(v, u)$ is an arc, and the *in-degree* of $u$ is the number of its in-neighbors. $X$ is *$d$-in-regular* if all vertices have in-degree $d$. If $X$ is both $d$-out-regular and $d$-in-regular, then we say $X$ is $d$-regular.

The *adjacency matrix* of a digraph $X = (V, \mathcal{A})$ is a $|V| \times |V|$ matrix $A$ with

$$A_{u,v} = \begin{cases} 1, & (u, v) \in \mathcal{A}, \\ 0, & (u, v) \notin \mathcal{A}. \end{cases}$$

Given an oriented graph $X = (V, \mathcal{A})$ and its adjacency matrix $A$, the *skew-symmetric adjacency matrix* of $X$ is $A - A^T$.

A *weighted digraph* is a digraph $X$ together with a function $\omega$ on the arcs; for an arc $(u, v)$, the value $\omega(u, v)$ is called the *weight* on $(u, v)$.

Given an $m \times m$ Hermitian matrix $H$, the *$H$-weighted digraph* is the digraph $X = (V, \mathcal{A})$ where

$$V = \{1, 2, \cdots, m\},$$

and

$$\mathcal{A} = \{(u, v) : H_{u,v} \neq 0\}$$

together with the weight $H_{u,v}$ assigned to the arc $(u, v)$. We call $H$ a *Hermitian adjacency matrix* of $X$.

Let $X = (V(X), E(X))$ and $Y = (V(Y), E(Y))$ be two graphs with adjacency matrices $A(X)$ and $A(Y)$. The *tensor product of $X$ and $Y$*, denoted $X \times Y$, is the graph with vertex set $V(X) \times V(Y)$, and two vertices $(u, a)$ and $(v, b)$ are adjacent in $X \times Y$ if

$$\{u, v\} \in E(X) \quad \text{and} \quad \{a, b\} \in E(Y).$$

The adjacency matrix of $X \times Y$ is given by the Kronecker product

$$A(X) \otimes A(Y).$$

The *Cartesian product of $X$ and $Y$*, denoted $X \square Y$, is the graph with vertex set $V(X) \times V(Y)$, and two vertices $(u, a)$ and $(v, b)$ are adjacent in $X \times Y$ if

$$\{u, v\} \in E(X) \quad \text{and} \quad a = b$$

or

$$u = v \quad \text{and} \quad \{a, b\} \in E(Y).$$

The adjacency matrix of $X \square Y$ is given by

$$A(X) \otimes I + I \otimes A(Y).$$

The *double graph* of $X$ is the graph with vertex set $V(X) \times \{1, 2\}$, and two vertices $(u, j)$ and $(v, k)$ are adjacent in the double graph if $\{u, v\}$ is in $E(X)$. The adjacency matrix of the double graph of $X$ is given by

$$A(X) \otimes J_2.$$

The notions of tensor product, Cartesian product and double graph can be extended to oriented graphs $X$ and $Y$, with adjacency matrices $A(X)$ and

$A(Y)$ replaced by the skew-symmetric adjacency matrices of $X$ and $Y$ in the definitions.

Let $\Gamma$ be a group, and $\mathcal{C}$ a subset of $\Gamma$. A *Cayley digraph over* $\Gamma$ *with connection set* $\mathcal{C}$, denoted $X(\Gamma, \mathcal{C})$, is a digraph with $\Gamma$ as its vertex set, and $(u, v)$ is an arc if $vu^{-1} \in \mathcal{C}$. If the connection set $\mathcal{C}$ is inverse-closed, then $X(\Gamma, \mathcal{C})$ is a graph, called a *Cayley graph*.

If $\Gamma$ is a finite abelian group, then the eigenvalues and eigenvectors of a Cayley digraph over $\Gamma$ are determined by the characters of $\Gamma$. The following theorem is a standard result; for references, see Godsil [25, Ch 12] and Lovasz [51].

**7.1.1 Theorem.** *Let* $\Gamma$ *be a finite abelian group. Let* $X = X(\Gamma, \mathcal{C})$ *be a Cayley digraph over* $\Gamma$, *with adjacency matrix* $A$. *For any character* $\chi$ *of* $\Gamma$, *we have*

$$A\chi = \left( \sum_{g \in \mathcal{C}} \chi(g) \right) \chi. \qquad \square$$

A *circulant digraph* is a Cayley digraph over a cyclic group $\mathbb{Z}_n$.

Given a graph $X$ with adjacency matrix $A$, the *characteristic polynomial of* $X$, denoted $\phi(X, t)$, is given by

$$\phi(X, t) := \det(tI - A).$$

Two vertices $u$ and $v$ of $X$ are *cospectral* if the vertex-deleted subgraphs $X \backslash u$ and $X \backslash v$ have the same characteristic polynomial, that is,

$$\phi(X \backslash u, t) = \phi(X \backslash v, t).$$

## 7.2 Quantum Theory

A *quantum system* is a Hilbert space $\mathcal{H}$. In this thesis, we are mostly concerned with finite-dimensional quantum systems. Let $\mathcal{H} = \mathbb{C}^m$ be the $m$-dimensional vector space over the complex numbers with the usual inner product

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

A *quantum state* is a vector in $\mathcal{H}$ of unit length.

An *observable* is a Hermitian matrix $H$ acting on $\mathcal{H}$. Let the spectral decomposition of $H$ be

$$H = \sum_r \lambda_r E_r,$$

where $\lambda_r$ is an eigenvalue of $H$, and $E_r$ is the orthogonal projection onto the eigenspace of $\lambda_r$. If the system is in state $x$, then a *measurement* of the observable $H$ returns value $\lambda_r$ with probability

$$\langle x, E_{\lambda_r} x\rangle.$$

In the case where $H$ has simple eigenvalues, the measurement can be described using an orthonormal basis of $\mathcal{H}$ consisting of the eigenvectors of $H$.

The only operations we can apply to an isolated quantum system, that is, a system that does not interact with the environment, are unitary operations. Let $\{v_1, v_2, \ldots, v_m\}$ be an orthonormal basis of $\mathcal{H}$. Let $U$ be a unitary matrix acting on $\mathcal{H}$. Given initial state $x$, applying $U$ changes the system state to $Ux$, and measuring in the basis $\{v_1, v_2, \ldots, v_m\}$ yields outcome $j$ with probability

$$|\langle v_j, Ux\rangle|^2.$$

In an open quantum system, however, the operations do not have to be unitary, and we must give a more general definition of quantum states, which may occur after non-unitary transformations. A *density matrix* is a positive semidefinite matrix $\rho$ with $\mathrm{tr}(\rho) = 1$. A *pure state* is represented by a rank-one density matrix $\rho$; in this case, $\rho = xx^*$ for some unit vector $x$ in $\mathcal{H}$. Thus, all states in an isolated quantum systems are pure. A *mixed state* is a probabilistic ensemble of pure states $\{(p_j, \rho_j) : j = 1, 2, \cdots, \ell\}$, and can be represented by a density matrix $\rho$ with rank greater than one:

$$\rho = p_1\rho_1 + \cdots + p_\ell \rho_\ell.$$

Let $\rho$ be the current state of the system. In the case where a unitary operation $U$ is applied, the state is changed to $U\rho U^*$, and the outcome of a measurement in the standard basis is $j$ with probability given by the trace inner product

$$\langle U\rho U^*, E_{jj}\rangle = \mathrm{tr}(U\rho U^* E_{jj}).$$

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