Quantum Walks on Embeddings

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Abstract

We construct a new type of quantum walk from orientable embeddings. Two infinite families of quantum walks built from self-dual embeddings exhibit interesting phenomena. First, their Hamiltonians are Hermitian adjacency matrices of sparse digraphs. Second, all these walks satisfy the stay-at-home property—the probability that the walk stays at the initial state tends to 1 as the size of graph goes to infinity.

1 Introduction

Quantum walks were shown to be universal for quantum computation [2, 9, 12]. The first model of discrete quantum walks was formally introduced by Aharonov et al [1]. Since then, different models have been studied [7, 11, 10] and compared [14, 8].

In this paper, we construct a new quantum walk from an orientable embedding of a graph. Roughly speaking, the walk is defined by two partitions of the arcs: one based on the faces, and one on the vertices. To illustrate the idea, we take the planar embedding of $K_4$ as an example. As shown in Figure 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 in Equation (1).

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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 1: A Planar Embedding of \(K_4\)

If \(\hat{M}\) is the matrix obtained from \(M\) by normalizing each column, then \(\hat{M}\hat{M}^T\) is the orthogonal projection onto \(\text{col}(M)\), and so

\[ 2\hat{M}\hat{M}^T - I \]

is the reflection about \(\text{col}(M)\). Similarly, if \(\hat{N}\) is the normalized arc-tail incidence matrix, then

\[ 2\hat{N}\hat{N}^T - I \]

is the reflection about \(\text{col}(N)\). Now

\[ U := (2\hat{M}\hat{M}^T - I)(2\hat{N}\hat{N}^T - I) \]

|      | \(f_0\) | \(f_1\) | \(f_2\) | \(f_3\) |
|------|----------|----------|----------|----------|
| (0, 1) | 1        | 0        | 0        | 0        |
| (0, 2) | 0        | 0        | 1        | 0        |
| (0, 3) | 0        | 0        | 0        | 1        |
| (1, 0) | 0        | 0        | 0        | 1        |
| (1, 2) | 1        | 0        | 0        | 0        |
| (1, 3) | 0        | 1        | 0        | 0        |
| (2, 0) | 1        | 0        | 0        | 0        |
| (2, 1) | 0        | 1        | 0        | 0        |
| (2, 3) | 0        | 0        | 1        | 0        |
| (3, 0) | 0        | 0        | 1        | 0        |
| (3, 1) | 0        | 0        | 0        | 1        |
| (3, 2) | 0        | 1        | 0        | 0        |
is a unitary matrix, which serves as the transition matrix of our quantum walk.

A quantum walk of the above type will be called a vertex-face walk. While such a walk has never been studied, it is closely related to the well-known coined walk, as we explain now. Let $R$ be the permutation matrix that swaps the tail and the head of each arc. Reversing all the arcs in the facial walks produces the other consistent orientation, with $RM$ being the new arc-face incidence matrix. This does not affect the embedding, but it changes the transition matrix to

$$(2RM(RM)^T - I)(2\tilde{N}\tilde{N}^T - I) = R(2\tilde{M}\tilde{M}^T - I)R(2\tilde{N}\tilde{N}^T - I).$$

Note that $R(2\tilde{N}\tilde{N}^T - I)$ is precisely the transition matrix of the coined walk on $X$, while $R(2\tilde{M}\tilde{M}^T - I)$ is precisely the transition matrix of the coined walk on the dual graph relative to the embedding. Therefore, each step of the vertex-face walk is equivalent to two steps of the coined walk, one on the original graph and one on its dual graph.

Apart from its connection to the coined walk, there is a lot more to explore with the vertex-face model. We motivate our study on the spectral side of $U$ by asking two questions. First, any unitary matrix $U$ can be written as

$$U = \exp(iH)$$

for some Hermitian matrix, called the Hamiltonian. In this way, a discrete quantum walk can be implemented as a continuous quantum walk, given that $H$ is sparse. Thus, we would like to know which embeddings provide sparse Hamiltonians $H$, or more precisely, adjacency matrices of sparse digraphs. The second question is about the limiting behavior on a class of quantum walks. In contrast to classical random walks, quantum walks may exhibit the “stay-at-home” property—the probability that the walk stays at the initial state goes to 1 as the size of the graph grows. Following Godsil’s paper on continuous quantum walks [4], we look for families of embeddings that satisfy the same property in the vertex-face walk. Both questions can be answered through spectral analysis on $U$, and two infinite families are found to manifest the desired phenomenon, as summarized below.

(i) For $n \equiv 0, 1 \pmod{4}$, the quantum walk for a self-dual embedding of $K_n$ has exactly three eigenvalues. Its Hamiltonian is the adjacency
matrix, up to a scalar, of a digraph $Z_n$ with $n(n-1)$ vertices, in-degree and out-degree $n-2$, and eigenvalues 0 and $\pm i\sqrt{n^2 - 2n}$. These embeddings satisfy the stay-at-home property.

(ii) For $n \equiv 0 \pmod{4}$, the quantum walk for the double cover $K_2 \times K_n$ of a self-dual embedding of $K_n$ has exactly four eigenvalues. Its Hamiltonian splits into two commuting adjacency matrices of digraphs, up to a scalar. One of these digraphs is the lexicographical product of $Z_n$ with $\overline{K_2}$. These embeddings also satisfy the stay-at-home property.

# 2 Transition Matrix

Consider an embedding $\mathcal{M}$ of a graph $X$ on some orientable surface. We can orient the faces consistently, that is, for each edge $\{a, b\}$ that is contained in two distinct faces $\{f_0, f_1\}$, the direction it receives in $f_0$ is opposite to the direction it received in $f_1$. Thus, every arc is used by exactly one face. The directed walk formed by all arcs in a face is called a facial walk. For an illustration, see the planar embedding of $K_4$ in Figure 1.

We say an arc $(a, b)$ is incident to a facial walk $f$ if $(a, b) \in f$, and it is incident to a vertex $u$ if $u = a$. Let $M$ be the arc-face incidence matrix, and $N$ the arc-tail incidence matrix. More often we will use the normalized matrices $\hat{M}$ and $\hat{N}$, which are obtained from $M$ and $N$ by normalizing each column, respectively. The vertex-face quantum walk is determined by the transition matrix

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

Before examining the entries of $U$, we have a few remarks on duality. Given an embedding $\mathcal{M}$ of $X$, the dual graph $X^*$ relative to $\mathcal{M}$ is a graph with the faces of $\mathcal{M}$ as its vertices, where two faces are adjacent if they have an edge in common. Naturally $\mathcal{M}$ gives rise to an embedding of $X^*$, denoted $\mathcal{M}^*$, on the same surface.

2.1 Lemma. If $U$ is the vertex-face transition matrix for $\mathcal{M}$, then $U^T$ is the vertex-face transition matrix for $\mathcal{M}^*$.

Now we move on to some properties of $U$. Unless otherwise specified, we will assume every face of $\mathcal{M}$ is bounded by a cycle. For ease of notation, let

$$P := \hat{M}\hat{M}^T$$
and

\[ Q := \hat{N}\hat{N}^T. \]

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.

2.2 Lemma. For any arc \((a, b)\), let \( f_{ab} \) denote the facial walk using \((a, b)\).

(i) The projections \( P \) and \( Q \) are doubly stochastic, and so

\[ U1 = U^T1 = 1. \]

(ii) For two arcs \((a, b)\) and \((u, v)\),

\[
P_{(a, b), (u, v)} = \begin{cases} \frac{1}{\deg(f_{ab})}, & \text{if } f_{ab} = f_{cd}, \\ 0, & \text{otherwise.} \end{cases}
\]

and

\[
Q_{(a, b), (u, v)} = \begin{cases} \frac{1}{\deg(a)}, & \text{if } a = u, \\ 0, & \text{otherwise.} \end{cases}
\]

(iii) For two arcs \((a, b)\) and \((u, v)\),

\[
(PQ)_{(a, b), (u, v)} = (QP)_{(u, v), (a, b)} = \begin{cases} \frac{1}{\deg(u)\deg(f_{ab})}, & \text{if } u \in f_{ab}, \\ 0, & \text{otherwise.} \end{cases}
\]

(iv) For two faces \( f \) and \( h \),

\[
(\hat{M}^TQ\hat{M})_{f, h} = \frac{1}{\sqrt{\deg(f)\deg(h)}} \sum_{w \in f \cap h} \frac{1}{\deg(u)}. \]

For two vertices \( u \) and \( v \),

\[
(\hat{N}^T P\hat{N})_{u, v} = \frac{1}{\sqrt{\deg(u)\deg(v)}} \sum_{f, u, v \in f} \frac{1}{\deg(f)}. \]

\[ \square \]
The above lemma allows us to write out the entries of $U$ explicitly. Moreover, if either $X$ of $X^*$ is regular, we have a simple expression for $\text{tr}(U)$.

2.3 Lemma. Consider an orientable embedding of $X$ with $p$ vertices, $q$ edges and $s$ faces. If either $X$ or $X^*$ is regular, then

$$
\text{tr}(U) = 2\left( \frac{ps}{q} - (p + s - q) \right).
$$

Proof. We have

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

where $P$ and $Q$ are projections. From (iii) in Lemma 2.2, we see that

$$
\text{tr}(PQ) = \sum_{(u,v)} \frac{1}{\deg(u)} \frac{1}{\deg(f_{uv})} = \sum_{f} \frac{1}{\deg(f)} \sum_{u \in f} \frac{1}{\deg(u)}.
$$

If $X$ is $d$-regular, then

$$
\text{tr}(PQ) = \frac{s}{d} = \frac{ps}{2q}.
$$

Hence

$$
\text{tr}(U) = 4 \text{tr}(PQ) - 2 \text{tr}(P) - 2 \text{tr}(Q) - \text{tr}(I)
= 2 \frac{ps}{q} - 2(\text{rk}(P) + \text{rk}(Q) - 2q)
= 2 \left( \frac{ps}{q} - (p + s - q) \right).
$$

The case where $X^*$ is regular follows from duality. 

We end this section by making sure we are dealing with irreducible quantum walks. A quantum walk is called 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 meet of the arc-face partition and the arc-tail partition is the trivial partition. 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.
2.4 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 $\pi_1 \wedge \pi_2$ is the discrete partition, an $\pi_1 \vee \pi_2$ 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 $\pi_1 \wedge \pi_2$ 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 $\pi_1 \vee \pi_2$. \qed

2.5 Corollary. A vertex-face walk on a connected graph is irreducible. \qed

In the rest of this paper we will assume $X$ is connected, in addition to that all face boundaries of $\mathcal{M}$ are cycles.

3 Spectral Decomposition

We now discuss the spectral decomposition of the transition matrix $U$, based on Section 3 of [15]. The eigenvalues of $U$ can be divided into three classes: the real eigenvalue 1, the real eigenvalue $-1$, and the complex eigenvalues with norm one. For each class, we explain how to obtain a basis for the associated eigenspace.

To start off, note that the 1-eigenspace of $U$ is the direct sum

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

3.1 Lemma. We have

$$\text{col}(P) \cap \text{col}(Q) = \text{span}\{1\}.$$ 

Proof. Any vector lying in this intersection must be constant on the arcs leaving each vertex, as well as constant on the arcs of each face. Since $X$ is connected, this vector must have constant entries. \qed

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3.2 Lemma. We have
\[ \ker(P) \cap \ker(Q) = \ker \begin{pmatrix} M^T \\ N^T \end{pmatrix}. \]
Moreover, if \( q \) is the number of edges of \( X \), and \( g \) is the genus of the surface \( X \) is embedded on, then the dimension of this vector space is \( q + 2g - 1 \).

Proof. The first statement is immediate. To see the second statement, note that
\[
\dim \left( \ker \begin{pmatrix} P \\ Q \end{pmatrix} \right) = 2q - \text{rk} \begin{pmatrix} P & Q \end{pmatrix} = 2q - \dim(\text{col}(P) + \text{col}(Q)) = 2q - (\text{rk}(P) + \text{rk}(Q) - \dim(\text{col}(P) \cap \text{col}(Q))) = 2q - \text{rk}(M) - \text{rk}(N) + 1 = q + 2g - 1. \]

3.3 Corollary. Suppose \( X \) has \( q \) edges, and the surface has genus \( g \). Then the multiplicity of the eigenvalue 1 of \( U \) is equal to \( q + 2g \).

For the remaining eigenvalues, the incidence relation between vertices and faces plays a central role in finding the eigenvectors. Since every face is bounded by a cycle, the vertex-face incidence matrix is precisely
\[ B := N^T M \]
We also define
\[ \hat{B} := \hat{N}^T \hat{M} \]
and call it the normalized vertex-face incidence matrix.

3.4 Lemma. The eigenvalues of \( \hat{B}^T \hat{B} \) lie between 0 and 1.

Proof. Note that
\[ \hat{B}^T \hat{B} = \hat{M}^T Q \hat{M}. \]
Since the columns of \( \hat{M} \) form an orthonormal set, the eigenvalues of \( \hat{B}^T \hat{B} \) interlace those of \( Q \).
Similar to the 1-eigenspace, we have a direct sum decomposition of the $(-1)$-eigenspace:

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

3.5 Lemma. The linear map $y \mapsto \hat{M}y$ is an isomorphism from $\text{ker}(\hat{B})$ to $\text{col}(P) \cap \text{ker}(Q)$, and the linear map $z \mapsto \hat{N}^Tz$ is an isomorphism from $\text{ker}(\hat{B}^T)$ to $\text{ker}(P) \cap \text{col}(Q)$.

Proof. We prove the first part of the statement. If

$$ \hat{B}y = 0, $$

then

$$ P\hat{M}y = \hat{N}By = 0. $$

Hence

$$ \hat{M}y \in \text{col}(P) \cap \text{ker}(Q). $$

Moreover, since $\hat{M}$ has full column rank, this map is injective. On the other hand, for any $x \in \text{col}(P) \cap \text{ker}(Q)$, there is some $y$ such that

$$ x = \hat{M}y $$

and

$$ 0 = Qx = \hat{N}\hat{B}y, $$

which implies that

$$ y \in \text{ker}(\hat{B}). $$

3.6 Corollary. Let $p$ be the number of vertices and $s$ the number of faces. The multiplicity of the eigenvalue $-1$ of $U$ is equal to

$$ p + s - 2 \text{rk}(B). $$

Finally, we compute the eigenvectors for each complex eigenvalue of $U$.

3.7 Lemma. Suppose $\lambda \in (0, 1)$ is an eigenvalue of $\hat{B}^T\hat{B}$. Choose $\zeta \in \mathbb{R}$ such that $\cos(\zeta) = 2\lambda - 1$. Let

$$ T := 2Q - I. $$
The linear map
\[ z \mapsto (T - e^{i\zeta} I) \hat{M} z \]
is an isomorphism from the \( \lambda \)-eigenspace of \( \hat{B}^T \hat{B} \) to the \( e^{i\zeta} \)-eigenspace of \( U \), and the linear map
\[ z \mapsto (T - e^{-i\zeta} I) \hat{M} z \]
is an isomorphism from the \( \lambda \)-eigenspace of \( \hat{B}^T \hat{B} \) to the \( e^{-i\zeta} \)-eigenspace of \( U \).

Proof. Suppose
\[ \hat{B}^T \hat{B} z = \lambda z. \]
Let \( y = \hat{M} z \). Then
\[ PQy = \lambda y. \]
It is straightforward to check that the subspace spanned by \( y \) and \( Ty \) is \( U \)-invariant:
\[ U (Ty \ y) = (Ty \ y) \begin{pmatrix} 0 & -1 \\ 1 & 2 \cos(\zeta) \end{pmatrix}. \]
Since
\[ \begin{pmatrix} 0 & -1 \\ 1 & 2 \cos(\zeta) \end{pmatrix} \]
has two eigenvalues \( e^{\pm i\zeta} \), we have
\[ U (T - e^{\pm i\zeta} I) y = e^{\pm i\zeta} y. \]
Moreover, as \( 0 < \lambda < 1 \),
\[ T - e^{\pm i\zeta} I \]
is invertible, whence the map
\[ z \mapsto (T - e^{\pm i\zeta} I) \hat{M} z \]
is injective.

In practice the eigenprojection turns out to be more useful than the eigenvectors, so we derive an expression below.
3.8 Corollary. Let $\lambda \in (0, 1)$ be an eigenvalue of $\hat{B}^T \hat{B}$ with eigenprojection $E_\lambda$. Let $T = 2Q - I$. If $\cos(\zeta) = 2\lambda - 1$ and $\theta_\pm = e^{\pm i\zeta}$, then the $\theta_\pm$-eigenprojections of $U$ are

\[ F_{\theta_+} = \frac{1}{2(1 - \lambda^2)}(T - \theta_+ I)\hat{M}E_\lambda\hat{M}^T(T - \theta_- I) \]

and

\[ F_{\theta_-} = \frac{1}{2(1 - \lambda^2)}(T - \theta_- I)\hat{M}E_\lambda\hat{M}^T(T - \theta_+ I), \]

respectively. \hfill \Box

3.9 Corollary. The multiplicities of the complex eigenvalues of $U$ sum to

\[ 2 \rk(B) - 2. \hfill \Box \]

4 Hamiltonian

Once the spectral decomposition of $U$ is given, say

\[ U = \sum_r \theta_r F_r, \]

we can define the Hamiltonian of $U$ to be

\[ H := \frac{1}{i} \sum_r \log(\theta_r) F_r, \]

where $0 \leq \log(\theta_r) < 2\pi i$ for all $\theta_r$. Since $U$ is real, its spectrum is closed under complex conjugation, so an alternative expression for $H$ is

\[ H = \pi F_{-1} + \frac{1}{i} \sum_{r:0<\log(\theta_r)<\pi i} \log(\theta_r)(F_r - F_r^T). \]

Further, using Lemma 3.8, we can write out the second term purely in terms of the spectral decomposition of $\hat{B}^T \hat{B}$.

4.1 Lemma. For each eigenvalue $\lambda \in (0, 1)$ of $\hat{B}^T \hat{B}$ with eigenprojection $E_\lambda$, let $\zeta \in (0, \pi)$ be such that $\cos(\zeta) = 2\lambda - 1$. Then the Hamiltonian of $U$ is

\[ H = \pi F_{-1} + i \sum_{\lambda \in (0, 1)} \frac{2\zeta}{\sin(\zeta)} (Q\hat{M}E_\lambda\hat{M}^T - \hat{M}E_\lambda\hat{M}^T Q). \]
Proof. Let $T = 2Q - I$. For each $\lambda$, let $\theta_{\pm} = e^{\pm i\zeta}$ and $K = \hat{M}E_\lambda\hat{M}^T$. Then

$$F_{\theta_+} - F_{\theta_-} = \frac{1}{2\sin^2(\zeta)}(\theta_+ - \theta_-)(TK - KT)$$

$$= \frac{2i}{\sin(\zeta)}(QK - KQ).$$

Combining the above with $\theta_{\pm} = e^{\pm i\zeta}$ yields the result. 

To efficiently implement the vertex-face walk as a continuous quantum walk, the Hamiltonian has to be sparse. Lemma 4.1 suggests that we can think of $H$ as a Hermitian adjacency matrix of some weighted digraph, called the Hamiltonian digraph, where the weights are either real or imaginary. Intuitively, the more eigenvalues $U$ has, the denser its Hamiltonian digraph tends to be, with more weights on the arcs. This motivates us to look at embeddings for which $U$ has few eigenvalues.

If $U$ has exactly two eigenvalues, then they have to be 1 and $-1$. In this case $P$ and $Q$ commute, and so $U$ is symmetric of order two. We show that a vertex-face walk of order two must arise from a Hamilton cycle embedding, that is, an embedding where every face is bounded by a Hamilton cycle.

4.2 Theorem. Let $\mathcal{M}$ be an orientable embedding of a connected graph $X$. If $U$ has exactly two eigenvalues, then $\mathcal{M}$ is a Hamilton cycle embedding.

Proof. Suppose the eigenvalues of $U$ are 1 and $-1$. Corollary 3.9 tells us that $\text{rk}(B) = 1$.

Thus each facial cycle must visit all vertices. 

The next case of interest is when $U$ has exactly three eigenvalues—one real and two complex. This can realized by self-dual embeddings of $K_n$, as discussed in the next section.

5 Three Eigenvalues

An embedding of a graph $X$ is called self-dual if the dual graph $X^*$ is isomorphic to $X$. In this section, we show that the transition matrix of a self-dual embedding of $K_n$ has exactly three eigenvalues. Moreover, the Hamiltonian
Figure 2: Hamiltonian Digraph of the Planar Embedding of $K_4$

digraph is sparse—it is a digraph on $n(n - 1)$ vertices with in-valency and out-valency $n - 2$. Figure 2 is the Hamiltonian digraph of the planar embedding of $K_4$.

The following result gives a number-theoretic condition for $K_n$ to have a self-dual embedding.

5.1 Theorem (White [13]). The complete graph $K_n$ has a self-dual orientable embedding if and only if $n \equiv 0, 1 \pmod{4}$.

We first observe that the vertices and faces of a self-dual embedding of $K_n$ form a symmetric 2-design.

5.2 Lemma. Let $\mathcal{M}$ be a self-dual orientable embedding of $K_n$. Then

$$B^T B = BB^T = I + (n - 2)J.$$ 

Proof. By duality we only need to prove one equality. Since each face contains $n - 1$ vertices, it avoids exactly one vertex. It follows that every two faces have $n - 2$ vertices in common. 

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5.3 Corollary. Let $\mathcal{M}$ be a self-dual orientable embedding of $K_n$. Then $\hat{B}^T\hat{B}$ has exactly two eigenvalues. More precisely,

(i) $1$ is an eigenvalue of $\hat{B}^T\hat{B}$, with eigenprojection

$$\frac{1}{n}J.$$

(ii) $\frac{1}{(n-1)^2}$ is an eigenvalue of $\hat{B}^T\hat{B}$, with eigenprojection

$$I - \frac{1}{n}J.$$

Proof. We have

$$\hat{B}^T\hat{B} = \frac{1}{(n-1)^2}B^TB.$$

For (i), simply note that $1$ is an eigenvector for both $I$ and $J$ with eigenvalues $1$ and $n$. For (ii), note that every vector $z$ orthogonal to $1$ is an eigenvector for $I$ and $J$ with eigenvalues $1$ and $0$. \qed

The next result follows from Lemma 3.5 and Lemma 3.7.

5.4 Theorem. If $U$ is the transition matrix of a self-dual embedding of $K_n$, then its eigenvalues are $1$ and $e^{\pm i\zeta}$, where

$$\cos(\zeta) = \frac{2}{(n-1)^2} - 1.$$ \qed

Now we characterize the Hamiltonian of $U$ and prove its Hamiltonian digraph is regular.

5.5 Theorem. Let $U$ be the transition matrix of a self-dual embedding of $K_n$. Then

$$U = \exp(\gamma(U^T - U)),$$

for some $\gamma \in \mathbb{R}$.

Proof. Choose $\zeta \in \mathbb{R}$ such that

$$\cos(\zeta) = \frac{2}{(n-1)^2} - 1.$$
According to Lemma 4.1,
\[ H = \frac{2i\zeta}{\sin(\zeta)}(Q\hat{M}\hat{E}^TM - \hat{M}\hat{E}^TQ), \]
where
\[ E = I - \frac{1}{n}J \]
is the eigenspace of \( \hat{B}^T\hat{B} \) for the eigenvalue \( \frac{1}{(n-1)^2} \). Since
\[ \hat{M}\hat{E}^T = P - \frac{1}{n(n-1)}J, \]
it follows that
\[ Q\hat{M}\hat{E}^T - \hat{M}\hat{E}^TQ = PQ - PQ = \frac{1}{4}(U^T - U). \]
Therefore the Hamiltonian is an imaginary multiple of \( U^T - U \).

5.6 Theorem. Let \( U \) be the transition matrix of a self-dual embedding of \( K_n \). Its Hamiltonian digraph has in-valency and out-valency \( n - 2 \), and eigenvalues \( 0 \) and \( \pm i\sqrt{n^2 - 2n} \).

Proof. Based on Lemma 2.2 (iii), for any two arcs \((a, b)\) and \((u, v)\), we have
\[ (PQ - QP)_{(a,b),(u,v)} = \begin{cases} 
\frac{1}{(n-1)^2}, & \text{if } u \in f_{ab} \text{ and } a \notin f_{uv}, \\
1/(n-1)^2, & \text{if } u \notin f_{ab} \text{ and } a \in f_{uv}, \\
0, & \text{otherwise}.
\end{cases} \]
Thus for
\[ (U^T - U)_{(a,b),(u,v)} \]
to be non-zero, we need both \( a \neq u \) and \( f_{ab} \neq f_{uv} \).

Now we count the positive and negative entries of any row of \( U^T - U \), say indexed by \((a,b)\). For any positive entry, we need a vertex \( u \) that is in \( f_{ab} \), and a neighbor \( v \) of \( u \) such that \( f_{(u,v)} \) misses \( a \). However, any face missing \( a \) has to contain all the other \( n - 1 \) vertices, whence it is uniquely determined and can contain only one outgoing arc of \( u \). Therefore the number of positive
entry is equal to the number of vertices in $f_{ab}$ other than $a$, that is, $n - 2$. Finally, since $U\mathbf{1} = U^T \mathbf{1} = \mathbf{1}$, there are as many negative entries as positive entries in a row of $U^T - U$.

The eigenvalues of the Hamiltonian digraph can be easily derived from the eigenvalues of $U$. 

Before moving on to four-eigenvalue case, we spend a section understanding covers of embeddings. This provides a natural way to “lift” nice vertex-face walks.

6 Quantum Walks on Covers

An arc-function of index $r$ of $X$ is a map $\phi$ from the arcs of $X$ into $\text{Sym}(r)$, such that $\phi(u, v) = \phi(v, u)^{-1}$. The fiber of a vertex $u$ is the set

$$\{(u, i) : i = 0, 1, \ldots, r - 1\}.$$

If we replace each vertex of $X$ by its fiber, and join $(u, i)$ to $(v, j)$ whenever $\phi(u, v)(i) = j$, 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 $(1, 2) \in \text{Sym}(2)$. Then the double cover $K_4^\phi$ is isomorphic to the cube, as shown in Figure 4.

![Figure 3: $K_4$](image)

![Figure 4: A double cover of $K_4$](image)

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. 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 covers, known as the voltage graphs. A voltage graph of $X$ is a $r$-fold cover $Y = X^\phi$, with a subgroup $G \leq \text{Sym}(r)$ of order $r$, and two additional requirements:

(i) $\phi$ is a map from the arcs of $X$ into $G$;

(ii) $V(Y) = V(X) \times G$ and $E(Y) = E(X) \times G$.

Voltage graphs correspond to normal covers [6], and have been extensively studied. We only state one property that voltage graphs satisfy; for more background, see [5].

6.1 Theorem (Gross and Tucker [5]). Let $C$ be a $k$-cycle in $X$. Let $Y = X^\phi$ be a voltage graph of order $r$. If $\phi(C)$ has order $\ell$, then the components of $F(C)$ 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.

6.2 Theorem. Let $Y = X^\phi$ be a voltage graph of $X$. Let $\rho$ be the partition of the arcs of $Y$, where each cell is the preimage of some arc of $X$. Let $\hat{S}$ be its normalized incidence matrix of $\rho$. Then

$$U_X = \hat{S}^T U_Y \hat{S}.$$ 

Proof. Write $U_Y$ as

$$U_Y = (2\hat{M}_Y \hat{M}_Y^T - I)(2\hat{N}_Y \hat{N}_Y^T - I).$$
Let $\sigma$ be the partition of the vertices of $Y$ into fibers, with normalized incidence matrix $\hat{K}$. It is not hard to verify that
\[ \hat{N}_Y \hat{K} = \hat{S} \hat{N}_X \]
and
\[ \hat{N}_Y^T \hat{S} = \hat{K} \hat{N}_X^T. \]
Thus $(\rho, \sigma)$ is an equitable partition of $\hat{N}_Y$ [3]. It follows that
\[ \hat{N}_Y \hat{K} \hat{K}^T = \hat{S} \hat{S}^T \hat{N}_Y. \] (2)
Since
\[ \hat{N}_X = \hat{S}^T \hat{N}_Y \hat{K}, \]
the projection onto its column space can be written as
\[
\hat{N}_X \hat{N}_X^T = \hat{S}^T (\hat{N}_Y \hat{K} \hat{K}^T) \hat{N}_Y^T \hat{S} \\
= \hat{S}^T (\hat{S} \hat{S}^T \hat{N}_Y) \hat{N}_Y^T \hat{S} \\
= \hat{S}^T \hat{N}_Y \hat{N}_Y^T \hat{S}.
\]
Applying a similar argument to the preimages of facial walks, we can show that
\[ \hat{M}_X \hat{M}_X^T = \hat{S}^T \hat{M}_Y \hat{M}_Y^T \hat{S}. \]
Thus,
\[ U_X = \hat{S}^T (2 \hat{M}_Y \hat{M}_Y^T - I) \hat{S} \hat{S}^T (2 \hat{N}_Y \hat{N}_Y^T - I) \hat{S}. \] (3)
Finally, from Equation [2] we see that
\[ \hat{S} \hat{S}^T \hat{N}_Y \hat{N}_Y^T = \hat{N}_Y \hat{K} \hat{K}^T \hat{N}_Y^T \]
is a symmetric matrix, and so $\hat{S} \hat{S}^T$ commutes with $\hat{N}_Y \hat{N}_Y^T$. Therefore, Equation [3] reduces to
\[ U_X = \hat{S}^T U_Y \hat{S}. \]

7 Four Eigenvalues

If $U$ has exactly four eigenvalues, then they must be 1, $-1$, and two complex eigenvalues $\theta_{\pm} = e^{\pm i \zeta}$. Thus
\[ H = \pi F_{-1} + \zeta (F_{\theta_+} - F_{\theta_-}), \]

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and the Hamiltonian digraph splits into two commuting digraphs. Throughout this section, we assume the following.

(i) \( X = K_n \), where \( n \) is divisible by 4.
(ii) \( \phi \) is the arc-function that sends every arc of \( X \) to \( (1, 2) \in \text{Sym}(2) \).
(iii) \( M_X \) is the self-dual embedding of \( K_n \).

We show that the embedding \( \mathcal{M}_Y \) of the cover \( Y = K_n^\phi \) gives a transition matrix with exactly four eigenvalues. Note that \( Y = K_2 \times K_n \).

To start, let \( \rho \) be the partition of the arcs of \( Y \), where each cell is the preimage of some arc of \( X \). Let \( \widehat{S} \) be the normalized incidence matrix of \( \rho \).

7.1 Lemma. We have \( \widehat{M}_Y = \widehat{S} \widehat{M}_X \).

Proof. Every facial cycle \( C \) in \( X \) has odd length \( n - 1 \), so \( \phi(C) = (1, 2) \) and \( C \) is lifted to a facial cycle of length \( 2(n - 1) \). It follows that every facial walk in \( Y \) containing arc \( ((u, i), (v, j)) \) will also contain the arc \( ((u, j), (v, i)) \). \( \square \)

The relation between the vertex-face incidence matrices of \( \mathcal{M}_X \) and \( \mathcal{M}_Y \) leads to the following.

7.2 Corollary. We have

\( i \) \( \widehat{B}_Y^T \widehat{B}_Y = \widehat{B}_X^T \widehat{B}_X \).

\( ii \) \( \widehat{B}_Y \widehat{B}_Y^T = \frac{1}{2(n - 1)} \widehat{B}_X \widehat{B}_X^T \otimes J_2 \).

Proof. The first part follows from the previous lemma and the fact about the quotient:

\( \widehat{S}^T \widehat{N}_Y \widehat{N}_Y^T \widehat{S} = \widehat{N}_X \widehat{N}_X^T \).

To see the second part, note that for any vertex \( u \) of \( X \), the vertex \( (u, 0) \) appears in a face \( f \) of \( Y \) if and only if \( (0, 1) \) appears in \( f \). By Corollary 5.2, 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 Lemma 2.2 (iv) yields the identity. \( \square \)
7.3 Corollary. We have the following.

(i) The complex eigenvalues of $U_Y$ are the same as the complex eigenvalues of $U_X$, with the same multiplicity.

(ii) $-1$ is an eigenvalue of $U_Y$. Moreover, the eigenspace is spanned by the vectors $x_u$ over all vertices $u$ of $X$, where $x_u$ 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 is clear from Corollary 7.2 (i) and Lemma 5.2. We also see that\[ \text{col}(P_Y) \cap \ker(Q_Y) = \{0\}. \]

Since each $x_u$ is constant on the outgoing arcs of each vertex if $Y$, and sum to zero over each face of $Y$, the set\[ \{x_u : u \in V(X)\} \]
forms an orthogonal basis of\[ \ker(P_Y) \cap \text{col}(Q_Y). \]

Our main result of this section is that the Hamiltonian digraph of $U_Y$ splits into two commuting sparse digraphs.

7.4 Theorem. There is a real $\alpha$ and an imaginary $\beta$ such that\[ U_Y = \exp(\alpha H_1 + \beta H_2), \]
where\[ H_1 = J_n \otimes \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \otimes J_{n-1}, \]
and\[ H_2 = U_T^T - U_Y = (U_T^T - U_X) \otimes J_2. \]

Proof. We have for some complex numbers $\theta_\pm = e^{\pm i \zeta}$ that\[ H = \pi F_{-1} + \zeta (F_{\theta_+} - F_{\theta_-}). \]

By Corollary 7.3 (ii), the eigenprojection $F_{-1}$ is a real multiple of $H_1$. From Lemma 4.1, Theorem 5.5 and Lemma 7.1, we see that $F_{\theta_+} - F_{\theta_-}$ is an imaginary multiple of\[ Q_Y \tilde{S} K \tilde{S}^T - \tilde{S} K \tilde{S}^T Q_Y, \]
where\[ K = P_X - \frac{1}{n(n-1)} J. \]

Applying Lemma 7.1 again yields the expression of $H_2$. \qed
One consequence of the above is that the Hamiltonian graph corresponding to $H_1$ is the lexicographical product of the Hamiltonian graph of $\mathcal{M}_X$ with $K_2$. Thus, it has in-valency and out-valency $2(n - 2)$, and eigenvalues $0$ and $\pm 2i/\sqrt{n^2 - 2n}$.

8 Stay-At-Home

One counterintuitive phenomenon on quantum walks is that a walk may be reluctant to leave its initial state. This property has been observed in continuous quantum walks on complete graphs, some cones and some strongly regular graphs [4]. Following this paper, we say a sequence of discrete quantum walks, determined by transition matrices $U_1, U_2, \ldots$, satisfies the stay-at-home property if for any time $k$, the mixing matrices $U_n^k \circ \overline{U_n^k}$ converge to $I$ as $n$ goes to infinity. Both families studied earlier exhibit this phenomenon.

8.1 Theorem. Let $U_n$ be the transition matrix of a self-dual embedding of $K_n$. The quantum walks determined by 

$$\{U_n : n \equiv 0, 1 \pmod{4}\}$$

satisfy the stay-at-home property.

Proof. The spectral decomposition of $U_n^k$ is 

$$U_n^k = F_1 + e^{ik}\zeta F_+ + e^{-ik}\zeta F_-,$$

where $F_\pm$ are the eigenprojections onto the eigenspaces of $e^{\pm i\zeta}$. Recall that 

$$\text{rk}(F_1) = (n - 2)(n - 1),$$

and 

$$\text{rk}(F_+) = \text{rk}(F_-) = n - 1.$$ 

Thus 

$$\text{tr}(U_n^k) = (n - 2)(n - 1) + 2\cos(k\zeta)(n - 1).$$

From Theorem 5.6 we see that $U_n$ has constant diagonal, which implies that $U_n^k$ has constant diagonal. Hence, each entry of $U_n^k \circ \overline{U_n^k}$ equals 

$$\left(1 - \frac{2 - 2\cos(k\zeta)}{n}\right)^2,$$

which converges to $1$ as $n$ goes to infinity. \hfill \Box
8.2 Theorem. Let $\mathcal{M}_X$ be a self-dual embedding of $X = K_n$. Let $\phi$ be the arc-function of $X$ that sends every arc to $(1, 2) \in \text{Sym}(2)$. Let $U_n$ be the transition matrix of the embedding $\mathcal{M}_Y$ of $Y = X^\phi$. If $n$ is divisible by 4, then the sequence $U_n$ satisfies the stay-at-home property.

Proof. The spectral decomposition of $U_n^k$ is
\[ U_n^k = F_1 + (-1)^k F_{-1} + e^{ik\zeta} F_+ + e^{-ik\zeta} F_- \]
Since
\[ \text{rk}(F_1) = 2(n - 1)^2 - n, \quad \text{rk}(F_{-1}) = n, \quad \text{rk}(F_\pm) = n - 1, \]
we have
\[ \text{tr}(U_n^k) = 2(n - 1)^2 - n + (-1)^k n + 2 \cos(k\zeta)(n - 1). \]
By 7.4 $U_n^k$ has constant diagonal, whence each entry of $U_n^k \circ U_n^k$ is
\[ \left(1 - \frac{2 - 2 \cos(k\zeta)}{2n} + \frac{(-1)^2 - 1}{2(n - 1)} \right)^2, \]
which converges to 1 as $n$ goes to infinity. \qed

9 Open Problems

We list some open problems that arise from this paper.

On the algebraic graph theoretic side, we would like to characterize the Hamiltonian digraphs of a vertex-face walk; in particular, a graph on $n(n-1)$ vertices with in-degree and out-degree $n-2$, and eigenvalues 0 and $\pm i\sqrt{n^2 - 2n}$.

On the topological graph theoretic side, we are interested in the following existence question: given an incidence structure with points $V$ and blocks $F$, is there an orientable embedding with $V$ as vertices and $F$ as faces? An answer to this could lead to more interesting families of vertex-face walks.

On the quantum side, problems such as perfect state transfer and uniform mixing have not been studied in this model. These could be quite rare, especially when the entries of $U$ are real; for example, the following is a necessary condition on the size of a graph for uniform mixing to occur.
Lemma. If $X$ admits uniform mixing, then the number of arcs of $X$ is a perfect square divisible by 4.

Proof. Since $U$ is real with constant row sum and column sum, $U^k$ is flat for some $k$ if and only if it is a multiple of a real regular Hadamard matrix. □

However, for walks with nice Hamiltonians, it is possible that some of the techniques from continuous quantum walks can be used to prove results on discrete quantum walks.

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