An infinite family of circulant graphs with perfect state transfer in discrete quantum walks

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Abstract
We study perfect state transfer in Kendon’s model of discrete quantum walks. In particular, we give a characterization of perfect state transfer purely in terms of the graph spectra, and construct an infinite family of 4-regular circulant graphs that admit perfect state transfer. Prior to our work, the only known infinite families of examples were variants of cycles and diamond chains.

1 Introduction

Discrete quantum walks were first introduced by Aharonov et al. [1] as a quantum analogue of classical random walks. Since then, various models of discrete quantum walks have been proposed [25,29,32]. In [7], Bose posed a scheme for using spin chains to transmit quantum states in quantum computers. Later, Christandl et al. [10,11] studied the problem of perfect state transfer in spin networks with respect to the XY-coupling model. Both continuous and discrete quantum walks were shown to be universal for quantum computation [9,28,33], for which quantum state transfer plays a role in implementing the universal quantum gate set. In particular, discrete perfect state transfer was first studied by Lovett et al. [28] on “wire” structures, where the quantum walk may propagate deterministically.

While there have been numerous results on perfect state transfer in continuous quantum walks [2–4,8,13,14,16,22,23,26], less is known on the discrete side, as the extra degree of freedom makes it harder to analyze the transition operator. Examples of perfect state transfer in discrete quantum walks have been found on simple structures. In [26], Kendon and Tamon showed that some diamond chains admit perfect state transfer between antipodal vertices. Kurzynski and Wojcik [27] found perfect state transfer on cycles, and discussed how to convert the position dependence of couplings

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into the position dependence of coins. Barr et al. [6] investigated discrete quantum walks on variants of cycles, and found some families such as $K_2 + C_n$ that admit perfect state transfer with appropriately chosen coins and initial states. In [34], Yalcinkaya and Gedik proposed a scheme to achieve perfect state transfer on paths and cycles using a recovery operator. With various setting of coin flippings, Zhan et al. [37] also showed that an arbitrary unknown two-qubit state can be perfectly transferred in one-dimensional or two-dimensional lattices. Recently, Stefanak and Skoupy analyzed perfect state transfer on stars [30] and complete bipartite graphs [31] 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 paper, we study perfect state transfer in a simple model proposed by Kendon [25], where each iteration consists of a Grover coin flip followed by an arc-reversal. We give a complete characterization of perfect state transfer in terms of graph spectra. Using this characterization, we construct an infinite family of 4-regular circulant graphs that admit perfect state transfer. Prior to our work, the only known infinite families of examples were variants of cycles and diamond chains.

2 Arc-reversal grover walks

We start by describing Kendon’s model of discrete quantum walks [25]. While her model applies to all graphs, we will focus on those that are regular.

Let $X$ be a $d$-regular graph on $n$ vertices. To construct a discrete quantum walk on $X$, we view $X$ as a directed graph, where each edge is replaced by a pair of opposite arcs. A quantum state associated with $X$ is a complex function on its arcs. These states form an inner product 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 [25], the transition matrix $U$ is defined to be a product of two sparse unitary matrices. Let $R$ be the permutation matrix that reverses each arc, and $G$ a $d \times d$ unitary matrix of the form

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

The transition matrix of the arc-reversal Grover walk on $X$ is

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

We will refer to $R$ as the arc-reversal operator, $G$ as the Grover coin, and $I \otimes G$ the coin operator.
3 Spectral decomposition of two-reflection walks

Notice that both $R$ and $I \otimes G$ are symmetric and have order two:

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

therefore, they represent reflections about subspaces. In [32], Szegedy studied the spectrum of a unitary matrix that is a product of two reflections. Later in Godsil’s unpublished notes [19], he developed some machinery toward finding the spectral decomposition of any matrix lying in the algebra generated by two reflections. We will summarize Godsil’s results in this section; the proofs are taken from Section 2.3 of Zhan’s Ph.D. thesis [36].

Let $P$ and $Q$ be two projection matrices acting on $\mathbb{C}^m$. Let $\langle P, Q \rangle$ denote the matrix algebra generated by $P$ and $Q$. The following well-known result enables us to diagonalize any matrix in $\langle P, Q \rangle$.

3.1 Lemma The vector space $\mathbb{C}^m$ 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 some vector $z$. Since $Pz \in W$ and $Qz \in W$, both $Pz$ and $Qz$ are scalar multiples of $z$, and so $z$ is a common eigenvector of $P$ and $Q$. Now, 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 nonzero eigenvalue, that is,

$$Qz = z.$$ 

Since

$$QPz = QPQz = 0,$$

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

For any matrix $N$, we use $\text{col}(N)$ to denote the column space of $N$. Let $U$ be the product of two reflections about $\text{col}(P)$ and $\text{col}(Q)$, that is,

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

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 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 $-1$. The 2-dimensional $\langle P, Q \rangle$-invariant subspaces provide eigenspaces for $U$ with non-real eigenvalues.

Since $P$ and $Q$ are positive-semidefinite, there are matrices $K$ and $L$ with orthonormal columns such that

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

Define

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

This matrix largely determines the spectrum of $U$.

**3.2 Lemma** The eigenvalues of $SS^*$ lie in $[0, 1]$. Let $y$ be an eigenvector for $SS^*$. Let $z = Ly$. We have the following correspondence between eigenvectors for $SS^*$ and eigenvectors for $U$.

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

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

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

$$z \in \text{ker}(P) \cap \text{col}(Q).$$
(iii) If \( y \) is an eigenvector for \( SS^* \) 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 \( SS^* \), that is, \( L^*PL \), interlace those of \( P \), which are 0 and 1. If

\[
L^*PLy = y,
\]

then

\[
y^*L^*(I - P)Ly = 0,
\]

and it follows from the positive-semidefiniteness of \( I - P \) that \( Ly \in \text{col}(P) \). 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 \(e^{\pm i\theta}\). \(\Box\)

**3.3 Lemma** The 1-eigenspace of \(U\) is the direct sum
\[
(\text{col}(P) \cap \text{col}(Q)) \oplus (\text{ker}(P) \cap \text{ker}(Q)),
\]
which has dimension
\[
m - \text{rk}(P) - \text{rk}(Q) + 2 \dim(\text{col}(P) \cap \text{col}(Q)).
\]
Moreover, the map \(y \mapsto Ly\) is an isomorphism from the 1-eigenspace of \(SS^*\) to \(\text{col}(P) \cap \text{col}(Q)\).

**Proof** If \(z\) is in \(\text{col}(P) \cap \text{col}(Q)\), then \(Pz = z\) and \(Qz = z\), so
\[
Uz = (2P - I)(2Q - I)z = z.
\]
If \(z\) is in \(\text{ker}(P) \cap \text{ker}(Q)\), then \(Pz = 0\) and \(Qz = 0\), so
\[
Uz = (2P - I)(2Q - I)z = -(-z) = z.
\]
By linearity, every vector in
\[
(\text{col}(P) \cap \text{col}(Q)) \oplus (\text{ker}(P) \cap \text{ker}(Q))
\]
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

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

For the multiplicity, note that

\[
\dim(\ker(P) \cap \ker(Q)) = \dim \left( \ker \begin{pmatrix} P \\ Q \end{pmatrix} \right)
= m - \text{rk}(P, Q)
= m - \dim(\text{col}(P, Q))
= m - \dim(\text{col}(P) + \text{col}(Q))
= m - (\text{rk}(P) + \text{rk}(Q) - \dim(\text{col}(P) \cap \text{col}(Q))).
\]

The isomorphism follows from Lemma 3.2. \( \square \)

**3.4 Lemma** The \((-1)\)-eigenspace of \( U \) is the direct sum

\[
(\text{col}(P) \cap \ker(Q)) \oplus (\ker(P) \cap \text{col}(Q)),
\]

which has dimension

\[
\text{rk}(P) + \text{rk}(Q) - 2 \text{rk}(S).
\]

Moreover, \( y \mapsto Ky \) is an isomorphism from \( \ker(S) \) to \( \text{col}(P) \cap \ker(Q) \), and \( y \mapsto Ly \) is an isomorphism from \( \ker(S^*) \) to \( \ker(P) \cap \text{col}(Q) \).

**Proof** The direct sum decomposition follows from a similar argument as the proof of Lemma 3.3, by replacing \( Q \) with \( I - Q \).

We now prove the two isomorphisms from \( \ker(S) \) to \( \text{col}(P) \cap \ker(Q) \) and from \( \ker(S^*) \) to \( \ker(P) \cap \text{col}(Q) \). As a consequence, the dimension of the \((-1)\)-eigenspace is

\[
(\text{rk}(P) - \text{rk}(S)) + (\text{rk}(Q) - \text{rk}(S)) = \text{rk}(P) + \text{rk}(Q) - 2 \text{rk}(S).
\]

First, suppose \( Sy = 0 \). Then,

\[
QKy = LSy = 0.
\]

Hence,

\[
Ky \in \text{col}(P) \cap \ker(Q).
\]

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

\[
z = Ky
\]
and

\[ 0 = Qz = LSy. \]

Thus,

\[ Sy = L^*LSy = L^*(LSy) = L^*0 = 0, \]

which implies that

\[ y \in \ker(S). \]

A similar argument shows that \( y \mapsto Ly \) is an isomorphism from \( \ker(S^*) \) to \( \ker(P) \cap \text{col}(Q) \).

### 3.5 Lemma

The dimensions of the eigenspaces for \( U \) with non-real eigenvalues sum to

\[ 2 \operatorname{rk}(S) - 2 \dim(\text{col}(P) \cap \text{col}(Q)). \]

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 the dimension formulas in Lemma 3.3 and Lemma 3.4, the orthogonal complement of the \((\pm1)\)-eigenspaces for \( U \) has dimension

\[ m - (m - \operatorname{rk}(P) - \operatorname{rk}(Q) + 2 \dim(\text{col}(P) \cap \text{col}(Q))) + \operatorname{rk}(P) + \operatorname{rk}(Q) - 2 \operatorname{rk}(S), \]

that is,

\[ 2(\operatorname{rk}(SS^*) - \dim(\text{col}(P) \cap \text{col}(Q))). \]

The isomorphisms now follow from Lemma 3.2. \( \square \)
4 Graph spectra versus walk spectra

We apply the previous results to the transition matrix of an arc-reversal Grover walk:

\[ U = R(I \otimes G). \]

While \( U \) is not defined in terms of the adjacency matrix \( A \) of the graph \( X \), we find a spectral correspondence between \( U \) and \( A \). More specifically, eigenvalues of \( A \) provide the real parts of eigenvalues of \( U \), and eigenvectors of \( A \) can be “lifted” to eigenvectors of \( U \) by two incidence matrices.

In what follows, for any arc \((u, v)\), we will refer to \( u \) as its tail, and \( v \) as its head.

To start, 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 \( e \) is an edge, then \((D_t)_{u,e} = 1\) if \( u \) is the tail of \( e \), and \((D_h)_{u,e} = 1\) if \( u \) is the head of \( e \).

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 \( e \).

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 endpoint of \( e \).

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

\[
D_t = \begin{pmatrix}
(0, 1) & (0, 2) & (1, 0) & (1, 2) & (2, 0) & (2, 1) \\
0 & 1 & 1 & 0 & 0 & 0 \\
1 & 0 & 0 & 1 & 1 & 0 \\
2 & 0 & 0 & 0 & 0 & 1 \\
\end{pmatrix}
\]

\[
D_h = \begin{pmatrix}
(0, 1) & (0, 2) & (1, 0) & (1, 2) & (2, 0) & (2, 1) \\
0 & 0 & 0 & 1 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 \\
2 & 0 & 1 & 0 & 0 & 0 \\
\end{pmatrix}
\]

\[
M = \begin{pmatrix}
(0, 1) & (0, 2) & (1, 2) \\
(0, 1) & 1 & 0 & 0 \\
(0, 2) & 0 & 1 & 0 \\
(1, 0) & 1 & 0 & 0 \\
(1, 2) & 0 & 0 & 1 \\
(2, 0) & 0 & 1 & 0 \\
(2, 1) & 0 & 0 & 1 \\
\end{pmatrix}
\]
Next, we list some useful identities about these incidence matrices. Let $A$ be the adjacency matrix of $X$.

4.1 Lemma We have

(i) $D_t D_t^T = D_h D_h^T = dI$
(ii) $M^T M = 2I$,
(iii) $D_t D_t^T = D_h D_h^T = A$,
(iv) $BB^T = A + dI$
(v) $D_t M = D_h M = B$,
(vi) $D_t R = D_h$,
(vii) $R = MM^T - I$, and
(viii) $I \otimes G = \frac{2}{d} D_t^T D_t - I$.

Proof We give a proof for (iii); the remaining identities can be verified in a similar manner. Let $E(X)$ denote the set of edges of $X$. For any two vertices $u$ and $v$ of $X$, we have

\[
(D_t D_h^T)_{uv} = \left( D_t^T e_u, D_h^T e_v \right) = \{ (a, b) : [a, b] \in E(X), \ a = u, \ b = v \} = \begin{cases} 1, & \{u, v\} \in E(X) \\ 0, & \{u, v\} \notin E(X). \end{cases}
\]

Hence, $D_t D_h^T = A$. Since $A$ is symmetric, we also have $D_h D_t^T = A$. \hfill \Box

As a consequence, $R$ is a reflection about $\text{col}(M)$, while $I \otimes G$ is a reflection about $\text{col}(D_t^T)$. We now apply Lemmas 3.3, 3.4 and 3.5 to prove the spectral relation between $U$ and $A$.

The following result, which follows from Lemma 3.5, shows that all eigenspaces of $U$ with non-real eigenvalues are completely determined by the eigenspaces of $A$ with eigenvalues in $(-d, d)$. It also gives a concrete description on how to “lift” eigenvalues and eigenvectors of $A$ to those of $U$.

4.2 Theorem Let $y$ be an eigenvector for $A$ with eigenvalue $\lambda \in (-d, d)$. Suppose $\lambda = d \cos(\theta)$ for some $\theta \in \mathbb{R}$. 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
\[ K := \frac{1}{\sqrt{2}} M, \quad L := \frac{1}{\sqrt{d}} D_1^T, \quad S := L^* K. \]

According to Lemma 3.5, eigenspace for \( U \) with non-real eigenvalues are determined by eigenspaces for
\[ SS^* = \frac{1}{2d} B B^T = \frac{1}{2d} (A + dI). \]

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 4.1, we see that
\[ ((\cos(\theta) + 1)I - (e^{\pm i\theta} + 1)P)Ly \]
is a scalar multiple of
\[ D_1^T y - e^{\pm i\theta} D_h^T y, \]
which is an eigenvector for \( U \) with eigenvalue \( e^{\pm i\theta} \). \( \square \)

After normalizing the eigenvectors, we obtain the eigenprojections for non-real eigenvalues of \( U \).

4.3 Corollary Let \( \lambda \) be an eigenvalue of \( A \) that is neither \( d \) nor \( -d \). Let \( E_\lambda \) be the orthogonal projection onto the \( \lambda \)-eigenspace of \( A \). Suppose \( \lambda = d \cos(\theta) \) for some \( \theta \in \mathbb{R} \). Then, the \( e^{i\theta} \)-eigenprojection of \( U \) is
\[ \frac{1}{2d \sin^2(\theta)} (D_1 - e^{i\theta} D_h)^T E_\lambda (D_1 - e^{-i\theta} D_h), \]
and the \( e^{-i\theta} \)-eigenprojection of \( U \) is
\[ \frac{1}{2d \sin^2(\theta)} (D_1 - e^{-i\theta} D_h)^T E_\lambda (D_1 - e^{i\theta} D_h). \]
Proof Every eigenvector $y$ for $A$ with eigenvalue $\lambda$ lies in $\text{col}(E_\lambda)$. By Theorem 4.2, $$(D_t - e^{i\theta} D_h)^T y$$ is an eigenvector for $U$ with eigenvalue $e^{i\theta}$. Let $\{e_1, \ldots, e_n\}$ be the standard basis for $\mathbb{C}^n$. Taking $y = E_\lambda e_1, \ldots, E_\lambda e_n$ yields a basis for the $e^{i\theta}$-eigenspace of $U$. Thus, the orthogonal projection onto the $e^{i\theta}$-eigenspace of $U$ is the sum of the rank-1 projections onto $$(D_t - e^{i\theta} D_h)^T E_\lambda e_1, \ldots, (D_t - e^{i\theta} D_h)^T E_\lambda e_n,$$ that is, a scalar multiple of $$(D_t - e^{i\theta} D_h)^T E_\lambda (D_t - e^{-i\theta} D_h).$$ Using Lemma 4.1, we find the scalar as follows: $$\langle (D_t - e^{i\theta} D_h)^T y, (D_t - e^{i\theta} D_h)^T y \rangle$$ $$= \langle y, (D_t - e^{-i\theta} D_h)(D_t - e^{i\theta} D_h)^T y \rangle$$ $$= \langle y, (D_tD_t^T - e^{-i\theta} D_h D_t^T - e^{i\theta} D_tD_t^T + D_h D_t^T) y \rangle$$ $$= 2 \langle y, (dI - \cos(\theta)A) y \rangle$$ $$= 2(d - \cos(\theta)\lambda) \langle y, y \rangle$$ $$= 2d(1 - \cos^2(\theta)) \langle y, y \rangle$$ $$= 2d \sin^2(\theta) \langle y, y \rangle.$$ Thus, the $e^{i\theta}$-eigenprojection is given by $$\frac{1}{2d \sin^2(\theta)} (D_t - e^{i\theta} D_h)^T E_\lambda (D_t - e^{-i\theta} D_h).$$ The $e^{-i\theta}$-eigenprojection can be obtained in a similar fashion. $\square$

We also characterize the $(\pm 1)$-eigenspaces of $U$. In particular, their multiplicities depend on the parameters of $X$. Let $\mathbf{1}$ denote the all-ones vector.

4.4 Lemma The $1$-eigenspace of $U$ is $$(\text{col}(M) \cap \text{col}(D_t^T)) \oplus (\text{ker}(M^T) \cap \text{ker}(D_t))$$ with dimension $$\frac{nd}{2} - n + 2.$$
Moreover, the projection onto \( \text{col}(M) \cap \text{col}(D_t^T) \) 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 \( A \).

**Proof** Let

\[
P := \frac{1}{2} MM^T, \quad Q := \frac{1}{d} D_t^T D_t, \quad S := \frac{1}{\sqrt{2d}} B.
\]

Notice that \( \text{col}(P) = \text{col}(M), \text{ker}(P) = \text{ker}(M^T), \text{col}(Q) = \text{col}(D_t^T), \) and \( \text{ker}(Q) = \text{ker}(D_t) \). By Lemma 3.3, the 1-eigenspace is the direct sum:

\[
(\text{col}(M) \cap \text{col}(D_t^T)) \oplus (\text{ker}(M^T) \cap \text{ker}(D_t)).
\]

It also follows from Lemma 3.3 that \( y \mapsto D_t^T y \) is an isomorphism from the \((2d)\)-eigenspace of \( BB^T \) to \( \text{col}(M) \cap \text{col}(D_t^T) \). By Lemma 4.1 (iv), the \((2d)\)-eigenspace of \( BB^T \) is the \( d \)-eigenspace of \( A \), and so

\[
\text{col}(M) \cap \text{col}(D_t^T) = D_t^T \text{col}(E_d).
\]

Since \( X \) is connected and \( d \)-regular, its largest eigenvalue \( d \) has multiplicity 1, and

\[
E_d = \frac{1}{n} J.
\]

Thus, the projection onto \( \text{col}(M) \cap \text{col}(D_t^T) \) is

\[
\frac{1}{d} D_t^T E_d D_t = \frac{1}{nd} J.
\]

Finally, since \( X \) has \( nd/2 \) edges and \( n \) vertices,

\[
\text{rk}(M) = nd/2, \quad \text{rk}(D_t^T) = n.
\]

By Lemma 3.3, the dimension of the 1-eigenspace of \( U \) is

\[
nd - \frac{nd}{2} - n + 2 = \frac{nd}{2} - n + 2.
\]

\[\square\]

**4.5 Lemma** If \( X \) is bipartite, the \((-1)\)-eigenspace of \( U \) is

\[
M \text{ker}(B) \oplus D_t^T \text{ker}(B^T)
\]
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 \( A \). If \( X \) is not bipartite, the \((-1)\)-eigenspace of \( U \) is
\[ M \ker(B), \]
with dimension
\[ \frac{nd}{2} - n. \]

**Proof** As before, let
\[ K := \frac{1}{\sqrt{2}} M, \quad L := \frac{1}{\sqrt{d}} D_t^T, \quad S := L^* K = \frac{1}{2d} B. \]

By Lemma 3.4, the \((-1)\)-eigenspace of \( U \) is
\[ (\col(P) \cap \ker(Q)) \oplus (\ker(P) \cap \col(Q)). \]

It also follows from Lemma 3.4 that \( y \mapsto My \) is an isomorphism from \( \ker(B) \) to \( \col(P) \cap \ker(Q) \), and \( y \mapsto D_t^T y \) is an isomorphism from \( \ker(B^T) \) to \( \ker(P) \cap \col(Q) \). Thus, the \((-1)\)-eigenspace of \( U \) is
\[ M \ker(B) \oplus D_t^T \ker(B^T). \]

Moreover, by Lemma 4.1(iv),
\[ \ker(B^T) = \ker(BB^T) = \ker(A + dI), \]
which is the eigenspace for \( A \) with eigenvalue \(-d\). Hence,
\[ \ker(B^T) = \col(E_{-d}). \]

Finally, by Lemma 3.4, the dimension of the \((-1)\)-eigenspace of \( U \) is
\[ \rk(M) + \rk(D_t) - 2 \rk(B) = \frac{nd}{2} + n - 2 \rk(B). \]
Since \( \text{rk}(B) = n - 1 \) if \( X \) is bipartite, and \( \text{rk}(B) = n \) otherwise, the dimension of the \((-1)\)-eigenspace of \( U \) is \( nd/2 - n + 2 \) if \( X \) is bipartite, and \( nd/2 - n \) otherwise. □

### 5 Perfect state transfer

In this section, we derive necessary and sufficient conditions for perfect state transfer to occur on arc-reversal Grover walks. 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 PhD thesis [12].

Suppose we start with a state that “concentrates on” \( u \), that is, a complex function that sends all but the outgoing arcs of \( u \) to zero. In theory, this state 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 \( u \):

\[
\frac{1}{\sqrt{d}} e_u \otimes 1.
\]

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

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

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 Grover walk, the only possible choice of \( x \) is

\[
\frac{1}{\sqrt{d}} 1,
\]

as we show now.

**5.1 Lemma** If \( X \) admits perfect state transfer from \( u \) to \( v \) at time \( k \), then

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

**Proof** Suppose

\[
U^k \left( \frac{1}{\sqrt{d}} e_u \otimes 1 \right) = e_v \otimes x.
\]

Since \( U \) has real entries, all entries in \( x \) are also real. Moreover, as \( 1 \otimes 1 \) is an eigenvector for \( U \) with eigenvalue 1,

\[
\left\langle 1 \otimes 1, \frac{1}{\sqrt{d}} e_u \otimes 1 \right\rangle = \left\langle 1 \otimes 1, U^k \left( \frac{1}{\sqrt{d}} e_u \otimes 1 \right) \right\rangle = \left\langle 1 \otimes 1, e_v \otimes x \right\rangle.
\]
Comparing the left-hand side to the right-hand side, we see that
\[
\left( \mathbf{1}, \frac{1}{\sqrt{d}} e_u \right) \left( \mathbf{1}, \mathbf{1} \right) = \left( \mathbf{1}, e_v \right) \left( \mathbf{1}, x \right),
\]
that is,
\[
\langle \mathbf{1}, x \rangle = \sqrt{d}.
\]
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 \( \mathbf{1} \).

Note that when perfect state transfer occurs, both the initial state and the final state lie in \( \text{col}(D_t^T) \), so we have an equivalent definition for perfect state transfer from \( u \) to \( v \) at time \( k \), that is,
\[
U^k D_t^T e_u = D_t^T e_v.
\]

Our characterization of perfect state transfer relies heavily on this observation.

**5.2 Lemma** Let \( \lambda = d \cos(\theta) \) be an eigenvalue of \( A \) that is neither \( d \) nor \(-d\). Let \( E_\lambda \) be the projection onto the \( \lambda \)-eigenspace of \( A \), 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 Corollary 4.3,
\[
2d \sin^2(\theta) D_t F_{\pm} D_t^T = D_t (D_t - e^{\pm i\theta} D_h) E_\lambda (D_t - e^{\mp i\theta} D_h) D_t^T
= (dI - e^{\pm i\theta} A) E_\lambda (dI - e^{\mp i\theta} A)
= d^2 |1 - e^{i\theta} \cos(\theta)|^2 E_\lambda
= d^2 \sin^2(\theta) E_\lambda.
\]

**5.3 Theorem** Suppose the spectral decomposition of \( A \) is
\[
A = \sum_\lambda \lambda E_\lambda.
\]
Then, \( X \) admit perfect state transfer from \( u \) to \( v \) at time \( k \) if and only if 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 $\lambda = d \cos(\frac{j\pi}{k})$ for some even integer $j$.
(iii) If $E_{\lambda}e_u = -E_{\lambda}e_v \neq 0$, then $\lambda = d \cos(\frac{j\pi}{k})$ for some odd integer $j$.

**Proof** 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 $r$,

$$e^{ik\theta_r} F_r D_t^T e_u = F_r D_t^T e_v. \quad (1)$$

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

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

By Lemma 4.4, this holds if and only if

$$\frac{1}{nd} JD_t^T e_u = D_t^T E_d e_u = D_t^T E_d e_v = \frac{1}{nd} JD_t^T e_v. \quad (2)$$

Since $JD_t^T e_u \neq 0$, Eq. (2) implies that

$$E_d e_u \neq 0$$

and

$$E_d e_u = \frac{1}{d} D_t D_t^T E_d e_u = \frac{1}{d} D_t D_t^T E_d e_v = E_d e_v.$$

Conversely,

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

implies Eq. (2). Clearly, $d = d \cos(0)$, which satisfies (ii).

Suppose $e^{i\theta_r} = -1$. By Lemma 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, Eq. (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 (1) says that
\[ e^{i k \theta_r} F_r D_t^{T} e_u = F_r D_t^{T} e_v. \]
By Lemma 5.2,
\[ D_t F_t D_t^{T} = \frac{d}{2} E_{\lambda}, \]  
so
\[ \frac{d}{2} E_{\lambda} e_v = D_t F_t D_t^{T} e_v = e^{i k \theta_r} D_t F_t D_t^{T} e_u = e^{i k \theta_r} \frac{d}{2} E_{\lambda} e_u, \]
or equivalently,
\[ e^{i k \theta_r} E_{\lambda} e_u = E_{\lambda} e_v. \]  
Conversely, given Eq. (4), we have
\[ E_{\lambda}(e^{i k \theta_r} e_u - e_v) = 0, \]
which implies
\[ \langle e^{i k \theta_r} e_u - e_v, E_{\lambda}(e^{i k \theta_r} e_u - e_v) \rangle = 0, \]
or by Eq. (3) and that $F_r^2 = F_r$,

$$\langle F_r D_1^T (e^{ik\theta_r} e_u - e_v), F_r D_1^T (e^{ik\theta_r} e_u - e_v) \rangle = 0,$$

from which we see

$$F_r D_1^T (e^{ik\theta_r} e_u - e_v) = 0,$$

and so Eq. (1) holds.

Since both $E_{\lambda} e_u$ and $E_{\lambda} e_v$ have real entries, it follows from Eq. (4) that Eq. (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 $e^{ik\theta_r} = -1$. $\square$

The three conditions in Theorem 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.

5.4 Corollary 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 $2k$. $\square$

Let $X$ be a graph with spectral decomposition

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

The eigenvalue support of a vertex $u$, defined by Godsil [18], 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 $X - u$. It is shown in [20] 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 5.3 gives necessary and sufficient conditions on $\psi_u(t)$ for $X$ to be periodic at $u$.

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 $z^k - 1$. 

$\square$
Proof Setting $u = v$ in Theorem 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

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

for some even integer $j$ (as indicated by Condition (ii)), or equivalently,

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

for some even integer $j$, or equivalently,

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

divides $z^k - 1$. \hfill \Box

Two vertices $u$ and $v$ of $X$ are cospectral if the vertex-deleted subgraphs $X \setminus u$ and $X \setminus v$ 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 $A$. Strong cospectrality has been thoroughly studied by Godsil and Smith [21]; we cite a useful characterization below.

5.6 Theorem Two vertices $u$ and $v$ are strongly cospectral if and only if the following hold.

(i) $u$ and $v$ are cospectral.
(ii) For every eigenvalue $\lambda$ of $A$, the vectors $E_\lambda e_u$ and $E_\lambda e_v$ are parallel. \hfill \Box

6 An infinite family

Conditions (ii) and (iii) in Theorem 5.3 lead us to consider regular graphs whose eigenvalues are given by real parts of $2k$th roots of unity. A circulant graph $X = X(Z_n, \{c_1, c_2, \ldots, c_d\})$ is a Cayley graph over $Z_n$ with connection set

$$\{c_1, c_2, \ldots, c_d\} \subseteq Z_n.$$

If $\psi$ is a character of $Z_n$, then $\psi$ is also an eigenvector for $A$ with eigenvalue

$$\psi(c_1) + \cdots + \psi(c_d).$$
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.

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

Proof The eigenvalues of $A$ are
\[
\lambda_j = e^{aj\pi/\ell} + e^{-aj\pi/\ell} + e^{bj\pi/\ell} + e^{-bj\pi/\ell} = 2 \cos\left(\frac{aj\pi}{\ell}\right) + 2 \cos\left(\frac{bj\pi}{\ell}\right),
\]
for $j = 0, 1, \ldots, 2n - 1$. Since $a + b = \ell$,
\[
\lambda_j = 2(1 + (-1)^j) \cos\left(\frac{aj\pi}{\ell}\right).
\]
Therefore, when $j$ is odd,
\[
\lambda_j = 0,
\]
and when $j$ is even,
\[
\lambda_j = 4 \cos\left(\frac{aj\pi}{\ell}\right).
\]
It follows that the multiplicity of the eigenvalue 0 is $\ell$.

We now check the parity condition in Theorem 5.3 for each eigenvector of $A$. 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 the vectors
\[
\{e_u - e_{u+\ell} : u = 0, 1, \ldots, \ell - 1\}
\]
form an orthogonal basis for $\ker(A)$, or equivalently, the eigenspace of 0. Thus, if $E_0$ is the projection onto the 0-eigenspace, then
\[
E_0 e_u = -E_0 e_{u+\ell},
\]
and since we can write 0 as
\[
0 = 4 \cos\left(\frac{\ell\pi}{2\ell}\right),
\]
Fig. 1 $X(Z_6, \{1, 2, 4, 5\})$

Fig. 2 $X(Z_{10}, \{1, 4, 6, 9\})$

Condition (iii) in Theorem 5.3 is satisfied.

Now, for any eigenvalue $\lambda_j \neq 0$, its eigenprojection $E_{\lambda_j}$ is orthogonal to $E_0$, so

$$E_{\lambda_j} e_u = E_{\lambda_j} e_{u+\ell},$$

and since

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

Condition (i) and (ii) in Theorem 5.3 are satisfied. \qed

Figures 1, 2, 3, 4, 5, and 6 are the first few examples in the infinite family with perfect state transfer between the marked vertices.

7 Open problems

In this paper, we gave a characterization of perfect state transfer in arc-reversal Grover walks, and constructed an infinite family of circulant graphs that exhibit this phe-
nomenon. However, many questions still remain open; we list a few, in the hope of finding more examples of 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 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, one might want to study graphs for which

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

is a factor of $x^k - 1$. In [35], 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 col($D_T^T$) that perfect state transfer can be characterized using graph spectra. In principle, 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 col($D_T^T$)? If so, can we characterize such perfect state transfer purely in terms of the spectral decomposition of $A$?

Finally, perfect state transfer is a rare phenomenon, partly because the eigenvalue support needs to satisfy a very strong condition. However, if we are interested in pretty good state transfer from $u$ to $v$, that is, for any $\epsilon > 0$, there is a time $k$ at which the probability of being on $v$ is $\epsilon$-close to 1, given initial state $e_u \otimes x$, then the eigenvalue conditions in Theorem 5.3 can be relaxed. Pretty good state transfer has been found in continuous quantum walks, see for example [5,15,17,24]. We would like to see discrete analogues.
(iii) Can we characterize pretty good state transfer in discrete quantum walks? Is there any graph with pretty good state transfer but without perfect state transfer?

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