Periodic Graphs

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Abstract

Let $X$ be a graph on $n$ vertices with adjacency matrix $A$ and let $H(t)$ denote the matrix-valued function $\exp(iAt)$. If $u$ and $v$ are distinct vertices in $X$, we say perfect state transfer from $u$ to $v$ occurs if there is a time $\tau$ such that $|H(\tau)_{u,v}| = 1$. If $u \in V(X)$ and there is a time $\sigma$ such that $|H(\sigma)_{u,u}| = 1$, we say $X$ is periodic at $u$ with period $\sigma$. We show that if perfect state transfer from $u$ to $v$ occurs at time $\tau$, then $X$ is periodic at both $u$ and $v$ with period $2\tau$. We extend previous work by showing that a regular graph with at least four distinct eigenvalues is periodic with respect to some vertex if and only if its eigenvalues are integers. We show that, for a class of graphs $X$ including all vertex-transitive graphs, if perfect state transfer occurs at time $\tau$, then $H(\tau)$ is a scalar multiple of a permutation matrix of order two with no fixed points. Using certain Hadamard matrices, we construct a new infinite family of graphs on which perfect state transfer occurs.

1 Introduction

Let $X$ be a graph with adjacency matrix $A$. We define the matrix function $H(t)$ by

$$H(t) := \exp(itA) := \sum_{n \geq 0} \frac{i^n A^n t^n}{n!}.$$
We note that \( t \) is a real variable

\[
H(t)^* = \exp(-iAt) = H(t)^{-1}
\]

and therefore \( H(t) \) is a unitary matrix. We have \( H(0) = I \) and

\[
H(s+t) = H(s)H(t).
\]

We say that graph is \textit{periodic with respect to the vector} \( z \) if there is a real number \( \tau \) such that \( H(\tau)z \) is a scalar multiple of \( z \). (Since \( H(t) \) is unitary, this scalar will have absolute value 1.) We say that \( X \) is \textit{periodic relative to the vertex} \( u \) if it is periodic relative to the standard basis vector \( e_u \) or, equivalently if there is a time \( \tau \) such that \( |H(\tau)_{u,u}| = 1 \). We say that \( X \) itself is \textit{periodic} if there is a time \( \tau \) such that \( H(\tau) \) is diagonal.

If there are basis vectors \( z_1, \ldots, z_n \) such that \( X \) is periodic with period \( \tau_r \) relative to the vector \( z_r \) for \( r = 1, \ldots, n \), then it follows that \( X \) is periodic, with period dividing the product of the \( \tau_i \)'s.

We say we have \textit{perfect state transfer} if there are distinct vertices \( u \) and \( v \) in \( X \) and a time \( \tau \) such that

\[
|H(\tau)_{u,v}| = 1.
\]

(If this holds then \( H(\tau)_{u,v} \) is the only non-zero entry in its row and column.)

Christandl, Datta, Dorlas, Ekert, Kay and Landahl \cite{3} prove that we have perfect state transfer between the end-vertices of paths of length one and two, and between vertices at maximal distance in Cartesian powers of these graphs. A graph exhibiting perfect state transfer between two vertices \( u \) and \( v \) models a network of quantum particles with fixed couplings, in which the state of the particle in \( u \) can be transferred to the particle in \( v \) without any information loss.

This paper is an attempt to extend some of the results in the above paper, and in the more recent work by Saxena, Severini and Shparlinski \cite{10}. We prove that a regular graph is periodic if and only if its eigenvalues are integers. We also show for a wide class of regular graphs (including all vertex-transitive graphs and all distance-regular graphs) that if perfect state transfer occurs, then there is a time \( \tau \) such that \( H(\tau) \) is a permutation matrix of order two with zero diagonal. (And hence the number of vertices in the graph must be even.) Finally we present a new infinite class of antipodal distance-regular graphs where perfect state transfer occurs.
2 Perfect State Transfer and Eigenvalues

In this section we set up some of our machinery, and present a criterion for
perfect state transfer. Our main tool is the spectral decomposition of a real
symmetric matrix. Let $\theta_1, \ldots, \theta_d$ be the distinct eigenvalues of $A$ and let $E_i$
denote the matrix that represents orthogonal projection onto the eigenspace
associated with $\theta_i$. Then if $f$ is complex function that is defined on the
eigenvalues of $A$, we recall that

$$f(A) = \sum_{r=1}^{m} f(\theta_r) E_r.$$  

In particular

$$H(t) = \sum_{r} \exp(it\theta_r) E_r.$$  

Note also that the scalars $f(\theta_r)$ are the eigenvalues of $f(A)$ and $\sum E_r = I$.

2.1 Theorem. If perfect state transfer from $u$ to $v$ occurs on $X$ at time $\tau$,
then $X$ is periodic relative to $u$ and $v$ at time $2\tau$, and for each quadruple $\theta_k$, $\theta_\ell$, $\theta_r$, $\theta_s$ of eigenvalues of $X$ with $\theta_r \neq \theta_s$

$$\frac{\theta_k - \theta_\ell}{\theta_r - \theta_s} \in \mathbb{Q}.$$  

Proof. We may assume without loss that $u$ and $v$ are the first and second
vertices of our graph $X$. Suppose that perfect state transfer from $u$ to $v$
occurs at time $\tau$. Since $H(t)$ is symmetric

$$H(\tau)_{u,v} = H(\tau)_{v,u}$$  

and their common value has norm 1. Since $H(t)$ is unitary it follows that we
may assume it has the form

$$H(\tau) = \begin{pmatrix} T & 0 \\ 0 & H_1 \end{pmatrix}$$  

where

$$T = \gamma \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$  

and \( \|ga\| = 1 \). Hence
\[
H(2\tau) = \begin{pmatrix} \gamma^2 I_2 & 0 \\ 0 & H_1^2 \end{pmatrix}.
\] (2.1)
This proves the first part of the theorem.

If \( e_1 \) denotes the first standard basis vector, then \( H(2\tau)e_1 = \gamma^2 e_1 \). By spectral decomposition,
\[
H(\tau)e_1 = \sum_r \exp(i\tau \theta_r) E_re_1
\]
and
\[
\xi e_1 = \sum_r \xi E_re_1.
\]
The non-zero vectors \( E_re_1 \) are orthogonal and so linearly independent, whence we deduce that
\[
\exp(it\theta_r) = \xi
\]
for all \( r \). It follows that, for all \( r \) and \( s \),
\[
\exp(i\tau(\theta_r - \theta_s)) = 1
\]
and that \( \tau(\theta_r - \theta_s) \) is an integral multiple of \( \pi \).

We will say that a graph satisfies the ratio condition if the conclusion of this lemma holds true. Christandl et al [3] state that the ratio condition is a necessary condition for perfect transfer on a path, and Saxena et al [10] showed that it is a necessary condition for a circulant graph to be periodic. We note the following consequence of the proof of the previous theorem.

**2.2 Corollary.** If \( X \) is periodic with respect to a vertex, then the ratio condition holds for the eigenvalues of \( X \).

**Proof.** If \( X \) is periodic with period \( \tau \) relative to some vector \( z \), we can apply the argument of the proof with \( z \) in place of \( z_1 \), and no other change.  

### 3 Regular Graphs

We note that any graph whose eigenvalues are integers is periodic. We prove the following converse. Saxena et al [10] derive this result for circulants, and we use some of their ideas.
3.1 Theorem. Let $X$ be a connected $k$-regular graph on $n$ vertices with at least four distinct eigenvalues. If the ratio condition holds, then the eigenvalues of $X$ are integers.

Proof. Our first observation appears in the work of Saxena, Severini and Shparlinski [10]. Suppose that the valency of $X$ is $k$ and let $\theta_1$ be an eigenvalue of $X$ not equal to $k$. As $k$ is an eigenvalue of $X$ and the ratio condition holds, we see that for any two eigenvalues $\theta_r$ and $\theta_s$ of $X$

$$\frac{\theta_r - k}{\theta_1 - k} \in \mathbb{Q}.$$ 

Therefore there are rational numbers $a_r, b_r$ such that

$$\theta_r = a_r \theta_1 + b_r. \quad (3.1)$$

From this we also see that if $X$ has a second rational eigenvalue not equal to $k$, then all eigenvalues of $X$ are rational, and consequently they are integers.

Let $k$ and $\theta_1, \ldots, \theta_d$ be the distinct eigenvalues of $A$ and let $m_r$ denote the multiplicity of $\theta_r$. If $v = |V(X)|$, then

$$vk = tr(A^2) = k^2 + \sum_r m_r b_r^2 + 2 \theta_1 \sum_r m_r a_r b_r + \theta_1^2 \sum_r m_r a_r^2,$$

Hence the minimal polynomial of $\theta_1$ over $\mathbb{Q}$ is quadratic. We denote the image of an element $a$ in $\mathbb{Q}(\theta_1)$ by $\overline{a}$ and observe that $\overline{a} = a$.

By the ratio condition, if $\theta$ is an eigenvalue of $X$ distinct from $k$, then

$$\frac{\theta - k}{\theta - k} = a$$

where $a$ is rational. Hence

$$a = \overline{a} = \frac{\overline{\theta} - k}{\overline{\theta} - k} = a^{-1}$$

and $a = \pm 1$. If $a = 1$, then $\theta = \overline{\theta}$, implying that $\theta$ is rational. If $a = -1$ then

$$\theta - k = k - \overline{\theta}$$

and therefore

$$\frac{1}{2}(\theta + \overline{\theta}) = k.$$

Since no eigenvalue of $X$ can be greater than $k$, we are forced to conclude

$$\theta = \overline{\theta} = k$$

and again $\theta$ is rational. \qed
Note that this proof does not require \( X \) to be regular, it is enough that the largest eigenvalue be an integer.

If \( X \) is a connected regular graph with two eigenvalues, then it is the complete graph \( K_n \) with eigenvalues \( n - 1 \) and \(-1\). If \( X \) has three eigenvalues then it must be strongly regular and then either its eigenvalues are integers, of \( X \) is a so-called conference graph on \( n \) vertices with valency \((n - 1)/2\) (whence \( n \) is odd) and its eigenvalues are \((n - 1)/2\) and

\[
\frac{1}{2}(-1 \pm \sqrt{n}).
\]

If a conference graph on \( n \) vertices is periodic with period \( t \), then there must be integers \( a, b, c \) and a complex number \( \phi \) of absolute value 1 such that the following equations hold:

\[
\frac{1}{2}(n - 1)i\pi t = 2\pi ia + \phi \\
\frac{1}{2}(\sqrt{n} - 1)i\pi t = 2\pi ib + \phi \\
-\frac{1}{2}(\sqrt{n} + 1)i\pi t = 2\pi ic + \phi.
\]

If we subtract the second equation from the first we get

\[i\pi t(n - \sqrt{n}) = 4\pi i(a - b)\]

and subtracting the third from the second gives

\[i\pi t\sqrt{n} = 2\pi i(b - c)\]

On dividing the second equation by the first we find that

\[\sqrt{n} - 1 = 2\frac{a - b}{b - c},\]

which implies that \( \sqrt{n} \) is rational. Thus we conclude that a connected regular graph with at most three eigenvalues is periodic if and only if its eigenvalues are integers.

3.2 Corollary. A connected regular graph is periodic if and only if its eigenvalues are integers.

Proof. Clearly a graph \( X \) is periodic if its eigenvalues are integers. Conversely, if \( X \) is periodic, the ratio condition holds. If \( X \) has at least four eigenvalues then its eigenvalues are integers by the previous theorem. If it has at most three eigenvalues then the claim follows by our remarks above.
4 Irregular Graphs

As noted by Christand et al [3], perfect state transfer occurs on the path on three vertices. Its eigenvalues are

$$-\sqrt{2}, 0, \sqrt{2}.$$ an thus the ratio condition does not force the eigenvalues to be integers. We can prove the following.

4.1 Lemma. If X is periodic then all its eigenvalues lie in a quadratic extension of Q. If the eigenvalues of X are not all integers, then they are all irrational if |V(X)| is even; if |V(X)| is odd then 0 is an eigenvalue, the remaining eigenvalues are irrational and X is bipartite.

Proof. Let $\theta_1, \ldots, \theta_n$ be the eigenvalues of $X$ and assume that the minimal polynomial of $\theta_1$ over $\mathbb{Q}$ has degree greater than two. Let $\sigma$ be an element of the Galois group of $\mathbb{Q}(\theta_1): \mathbb{Q}$ and suppose $\theta_1^\sigma \neq \theta_1$.

By the ratio condition

$$\frac{\theta_1^{\sigma^2} - \theta_1^\sigma}{\theta_1^\sigma - \theta} \in \mathbb{Q}$$

and therefore there is $c$ in $\mathbb{Q}$ such that

$$(\theta_1^\sigma - \theta)^\sigma = c(\theta_1^\sigma - \theta).$$

If $\sigma$ has order $k$, then $c^k = 1$ and $c = \pm 1$.

If $c = -1$ then

$$\theta_1^{\sigma^2} - \theta_1^\sigma = \theta_1 - \theta_1^\sigma$$

and $\theta^{\sigma^2} = \sigma$. It follows that any non-identity element of the Galois group has order two, and therefore the Galois group is elementary abelian.

If $c = 1$ then

$$\theta_1^{\sigma^2} = 2\theta_1^\sigma - \theta_1$$

and so

$$\begin{pmatrix} \theta_1^{\sigma^2} \\
\theta_1^\sigma \end{pmatrix} = \begin{pmatrix} 2 & -1 \\
1 & 0 \end{pmatrix} \begin{pmatrix} \theta_1^\sigma \\
\theta_1 \end{pmatrix}. $$

Let $M$ denote the $2 \times 2$ coefficient matrix here. Then $M$ represents the action of $\sigma$ on the rational vector space spanned by $\theta_1$ and $\theta_1^\sigma$. A simple calculation shows that

$$M^k = \begin{pmatrix} k + 1 & -k \\
k - 1 & -k + 1 \end{pmatrix}.$$
and thus the order of $M$ is infinite. Since $\sigma$ has finite order, we conclude that we cannot have $c = 1$.

Let $\sigma$ and $\tau$ denote two elements of the Galois group of $\mathbb{Q}(\theta_1)/\mathbb{Q}$, where $\sigma \neq 1$. Since

$$\frac{\theta^\tau_1 - \theta_1}{\theta^\sigma_1 - \theta_1} \in \mathbb{Q}$$

we have

$$\theta^\tau_1 - \theta_1 = b(\theta^\sigma_1 - \theta_1)$$

for some rational $b$, and consequently the rational vector space spanned by $\theta^\tau_1$ and $\theta_1$ is invariant under the Galois group of $\mathbb{Q}(\theta_1) : \mathbb{Q}$. Since the Galois group is abelian, this implies that $\mathbb{Q}(\theta_1)$ is a quadratic extension.

Now let $\bar{\theta}_i$ denote the unique algebraic conjugate of $\theta_i$. Then

$$\frac{\bar{\theta}_i - \theta_i}{\theta_1 - \theta_1} \in \mathbb{Q}$$

and therefore there is $c$ in $\mathbb{Q}$ such that

$$\bar{\theta}_i - \theta_i = c(\bar{\theta}_1 - \theta_1).$$

Since $\bar{\theta}_i + \theta_i$ is an integer, it follows that

$$\theta_i = a + b(\bar{\theta}_1 - \theta_1)$$

for suitable rationals $a$ and $b$. This proves the first claim in the theorem.

The argument in the proof of Theorem 3.1 shows that if the ratio condition holds and $X$ has two (distinct) rational eigenvalues then its eigenvalues are all integers. Hence either $|V(X)|$ has an even number of vertices and all its eigenvalues are irrational, or $|V(X)|$ is odd and it has just one integer eigenvalue.

Suppose $|V(X)|$ is odd and $\ell$ is an integer eigenvalue. If $\theta$ is an irrational eigenvalue with algebraic conjugate $\bar{\theta}$, then

$$\frac{\bar{\theta} - \ell}{\theta - \ell} \in \mathbb{Q}$$

and therefore

$$\bar{\theta} - \ell = c(\theta - \ell)$$

(4.1)
for some rational $c$. Hence

$$(\theta - \ell)^{\sigma_k} = c^k(\theta - \ell)$$

and so $c^m = 1$ for some positive integer $m$. Thus again $c = \pm 1$. If $c = 1$, then Equation (4.1) implies that $\bar{\theta} = \theta$ and we have a second rational eigenvalue. So $c = -1$ and

$$\bar{\theta} + \theta = 2\ell.$$ 

Now the sum of the eigenvalues of $X$ is zero, but from the above this sum is equal to $|V(X)|\ell$. Consequently $\ell = 0$. Since this implies that the spectrum of $X$ is symmetric about zero, $X$ must be bipartite.

It is shown in [3] that perfect state transfer occurs between vertices of maximum distance in the Cartesian powers of the path $P_3$ on three vertices. The eigenvalues of the $k$-th Cartesian power are the numbers $(k - i)\sqrt{2}$ for $i = 0, \ldots, 2k$. It is easy to verify that these graphs are periodic.

## 5 Monomial Matrices

Recall that a monomial matrix is the product of a diagonal matrix and a permutation matrix—thus it is a square matrix with at most one non-zero entry in each row and column. An invertible monomial matrix is unitary if and only if each non-zero entry has absolute value 1.

One way of realizing perfect state transfer is to choose $X$ and $\tau$ such that $H(\tau)$ is monomial, but not diagonal.

### 5.1 Lemma. Let $X$ be a connected graph. If $H_X(\tau)$ is monomial, then it is a scalar multiple of a permutation matrix with order two and $X$ is periodic with period $2\tau$.

**Proof.** We claim that if $H(t)$ is monomial and $X$ is connected, then $H(t)$ is a scalar multiple of a permutation matrix. For if $H(t)$ is monomial, say $H(t) = DP$ where $P$ is a permutation matrix and $D$ is diagonal (and unitary), then since $H(t)$ commutes with $A$, we have $ADP = DPA$. Hence

$$P^{-1}D^{-1}ADP = A$$

and so

$$D^{-1}AD = PAP^{-1}.$$
Since $P$ is a permutation matrix, $PAP^{-1}$ is a 01-matrix and it follows that $D$ must be a scalar matrix.

So we suppose that $H(t) = \gamma P$, where $P$ is a permutation matrix. As $P$ is a complex polynomial in $A$ and $A$ is symmetric, so is $P$, and therefore $P^2 = I$. \hfill \Box$

Let say that a permutation matrix $P$ is realizable if $H(t)$ is scalar multiple of $P$ at some time $t$. We observe that the set of realizable permutation matrices forms a group, necessarily elementary abelian. Since each element of this group can be written as a polynomial in $A$, this group must be a subgroup of the centre of the automorphism group of $X$.

6 Coherent Algebras

A coherent algebra is a real or complex algebra of matrices that contains the all-ones matrix $J$ and is closed under Schur multiplication, transpose and complex conjugation. (The Schur product $A \circ B$ of two matrices $A$ and $B$ with same order is defined by

$$(A \circ B)_{i,j} = A_{i,j}B_{i,j}.$$ 

It has been referred to as the “bad student’s product”.) A coherent algebra always has a basis of 01-matrices and this is unique, given that its elements are 01-matrices. This set of matrices determines a set of directed graphs and the combinatorial structure they form is known as a coherent configuration. When we say that a graph $X$ is a “graph in a coherent algebra”, we mean that $A(X)$ is a sum of distinct elements of the 01-basis.

A coherent algebra is homogeneous if the identity matrix is an element of its 01-basis. If $M$ belongs to a homogeneous coherent algebra, then

$$M \circ I = \mu I$$ 

for some scalar $\mu$. Hence the diagonal of any matrix in the algebra is constant. If $A$ is a 01-matrix in the algebra, the diagonal entries of $AAT^T$ are the row sums of $A$. Therefore all row sums and all column sums of any matrix in the 01-basis are the same, and therefore this holds for each matrix in the algebra. In particular we can view the non-identity matrices as adjacency matrices of regular directed graphs. Any directed graph in a homogeneous coherent algebra must be regular.
We consider two classes of examples. First, if $\mathcal{P}$ is a set of permutation matrices of order $n \times n$, then the commutant of $\mathcal{P}$ in $\text{Mat}_{n \times n}(\mathbb{C})$ is Schur-closed. Therefore it is a coherent algebra, and this algebra is homogeneous if and only the permutation group generated by $\mathcal{P}$ is transitive.

For second class of examples, if $X$ is a graph we define the $r$-th distance graph $X_r$ of $X$ to be the graph with $V(X_r) = V(X)$, where vertices $u$ and $v$ are adjacent in $X_r$ if and only if they are at distance $r$ in $X$. So if $X$ has diameter $d$, we have distance graphs $X_1, \ldots, X_d$ with corresponding adjacency matrices $A_1, \ldots, A_d$. If we use $A_0$ to denote $I$, then the graph $X$ is distance regular if the matrices $A_0, \ldots, A_d$ are the 01-basis of a homogeneous coherent algebra. (It must be admitted that this is not the standard definition.) We will refer to the matrices $A_i$ as distance matrices.

A commutative coherent algebra is the same thing as a Bose-Mesner algebra of an association scheme. We will not go into this here, but we do note that the coherent algebra belonging to a distance-regular graph is commutative.

6.1 Theorem. If $X$ is a graph in a coherent algebra with vertices $u$ and $v$, and perfect state transfer from $u$ to $v$ occurs at time $\tau$, then $H(\tau)$ is a scalar multiple of a permutation matrix with order two and no fixed points that lies in the centre of the automorphism group of $X$.

Proof. First, if $A = A(X)$ where $X$ is a graph in a homogeneous coherent algebra then, because it is a polynomial in $A$, the matrix $H(t)$ lines in the algebra for all $t$. Hence if

$$|H(\tau)_{u,v}| = 1$$

it follows that $H(\tau) = \xi P$ for some complex number $\xi$ such that $|\xi| = 1$ and some permutation matrix $P$. Since $A$ is symmetric, so is $H(t)$ for any $t$, and therefore $P$ is symmetric. So

$$P^2 = PP^T = I$$

and $P$ has order two. Since $P$ has constant diagonal, its diagonal is zero and it has no fixed points. As $P$ is a polynomial in $A$, it commutes with any automorphism of $X$ and hence is central. \qed

6.2 Corollary. If $X$ is a graph in a coherent algebra with vertices $u$ and $v$ and perfect state transfer from $u$ to $v$ occurs at some time, then the number of vertices of $X$ is even.
Proof. Since $P^2 = I$ and the diagonal of $P$ is zero, the number of columns of $P$ is even.

Saxena et al. [10] proved this corollary for circulant graphs. A homogeneous coherent algebra is \textit{imprimitive} if there is a non-identity matrix in its 01-basis whose graph is not connected, otherwise it is \textit{primitive}. If the algebra is the commutant of a transitive permutation group, it is imprimitive if and only the group is imprimitive as a permutation group. The above corollary implies that if perfect state transfer takes place on a graph from a homogeneous coherent algebra, the algebra is imprimitive.

Note that our corollary holds for any vertex-transitive graph, and for any distance-regular graph.

7 Walk-Regular Graphs

A graph $X$ with adjacency matrix $A$ is \textit{walk regular} if the diagonal entries of $A^k$ are constant for all non-negative integers $k$. The terminology arises because if $X$ is walk regular and $r \geq 0$, the number of closed walks of length $r$ that start at a vertex $u$ is independent of $u$. Any vertex-transitive graph is walk regular; more generally any graph in a coherent algebra is walk regular. (However the converse does not hold, as will be shown by the example below.) A connected regular graph with at most four distinct eigenvalues is walk regular (see Van Dam [12]). Note that a walk-regular graph is necessarily regular.

7.1 Theorem. Suppose $X$ is a walk-regular graph with distinct vertices $u$ and $v$ such that perfect state transfer from $u$ to $v$ occurs at time $\tau$. Then $X$ is periodic with period $2\tau$.

Proof. We have seen that if perfect state transfer occurs at time $\tau$, then two of the diagonal entries of $H(2\tau)$ have norm 1. Since $H$ is walk regular, it follows that $H(2\tau)$ is a scalar matrix.

We have not been able to prove that if perfect state transfer occurs at time $\tau$ on $X$ and $X$ is walk regular, then $H_X(2\tau)$ is a scalar multiple of a permutation matrix. There seems to be no obvious reason to expect that this should be the case.

The graph in Figure 1 is walk regular but not vertex transitive. (The string below the graph in the figure is the graph6 string that describes the
This graph does not lie in a homogeneous coherent algebra—the row sums of the Schur product
\[ A \circ (A^2 - 4I) \circ (A^2 - 4I - J) \]
are not all the same.

Suppose \( X \) is walk regular and that perfect state transfer from \( u \) to \( v \) occurs at time \( \tau \). Then \( |H(\tau)_{u,v}| = 1 \) and consequently \( H(\tau)_{u,u} = 0 \). Since \( X \) is walk regular, the diagonal entries of \( H(\tau) \) are all equal and thus they are all zero. If \( m_\theta \) denotes the multiplicity of the eigenvalue \( \theta \), then
\[
\text{tr}(H(t)) = \sum_\theta m_\theta \exp(it\theta)
\]
and thus we may define the Laurent polynomial \( \mu(z) \) by
\[
\mu(z) := \sum_\theta m_\theta z^\theta.
\]
Here \( z = \exp(it) \) and we have made use of the fact that \( X \) is periodic and hence its eigenvalues are integers. We call \( \mu(z) \) the multiplicity enumerator of \( X \).
7.2 Lemma. Let $X$ be a walk-regular graph with integer eigenvalues. If perfect state transfer occurs on $X$, then $\mu(z)$ has an eigenvalue on the unit circle of the complex plane.

Proof. The trace of $H(t)$ is zero if and only if $\mu(\exp(it)) = 0$. \hfill \Box

The characteristic polynomial of the graph in Figure 1 is

$$(t - 4)(t - 2)^3 t^3 (t + 2)^5$$

and its multiplicity enumerator is

$$\mu(z) = z^{-2}(z^6 + 3z^4 + 3z^2 + 5).$$

This polynomial has no roots on the unit circle, and we conclude that perfect state transfer does not occur.

For more information on walk-regular graphs, see [5]. The computations in this section were carried out in sage [11]. Van Dam [12] studies regular graphs with four eigenvalues, as we noted these provide examples of walk-regular graphs.

8 Hypercubes

The $n$-cube was one of the first cases where perfect state transfer was shown to occur (see [3]). The $n$-cube is an example of a distance-regular graph, and in this section we establish some of the consequences of our work for distance-regular graphs.

Suppose $X$ is a distance-regular graph with diameter $d$ and distance matrices $A_0, \ldots, A_d$. It has long been known that if $X$ is imprimitive then either $X_2$ is not connected or $X_d$ is not connected (see [11] Chapter 22 or [2] Section 4.2]). For the $n$-cube, neither $X_2$ nor $X_n$ are connected. If $X_2$ is not connected then $X$ is bipartite and $X_m$ is not connected if $m$ is even. Here we will be concerned with the case where $X_d$ is not connected. In this case it follows from the work just cited that the components of $X_d$ must be complete graphs of the same size, and that two vertices of $X$ lie in the same component of $X_d$ if and only if they are at distance $d$ in $X$. The components are called the antipodal classes of $X$; note these may have size greater than two. If $X_d$ is not connected, we say that $X$ is an antipodal distance regular graph.

As already noted the $n$-cubes provide natural examples of distance-regular graphs. The $n$-cube has diameter $n$, and its vertices can be partitioned into
pairs such that two vertices in the same pair are at distance \( n \), while vertices in different pairs are at distance less than \( n \), hence it is antipodal.

Our next lemma is more or less a specialization of Corollary 6.2 to the case of distance-regular graphs.

**8.1 Lemma.** Suppose \( X \) is a distance-regular graph with diameter \( d \). If perfect state transfer from \( u \) to \( v \) occurs at time \( \tau \), then \( X \) is antipodal with antipodal classes of size two and \( H(\tau) = X_d \). \hfill \Box

We outline a proof that perfect state transfer occurs on the \( n \)-cube. In the following section we will use much the same argument to provide a second infinite class of examples.

The \( n \)-cube gives rise to an association scheme, that is, a commutative coherent configuration as follows. Let \( X \) be the graph of the \( n \)-cube, and view its vertices as binary vectors of length \( n \). Let \( X_i \) be the graph with the same vertex set as \( X \), where two vertices are adjacent if and only if they differ in exactly \( i \) positions. Thus \( X_1 = X \) and two vertices are adjacent in \( X_i \) if and only they are at distance \( i \) in \( X \). Let \( A_i \) be the adjacency matrix of \( X_i \) and set \( A_0 = I \). Then \( A_0, \ldots, A_n \) are symmetric 01-matrices and

\[
\sum_{r=0}^{n} A_r = J.
\]

It is known that these matrices commute and that their span is closed under matrix multiplication. Hence they form a basis for a commutative coherent algebra of dimension \( d + 1 \). Since this algebra is commutative and semisimple, it has a second basis \( E_0, \ldots, E_n \) of matrix idempotents. These are real symmetric matrices such that \( E_i E_j = \delta_{i,j} \) and

\[
\sum_{i=0}^{n} E_i = I.
\]

These idempotents represent orthogonal projection onto the eigenspaces of the algebra and hence there are scalars \( p_i(j) \) such that \( A_i E_j = p_i(j) E_j \). Consequently

\[
A_i = A_i I = A_i \sum_{r=0}^{n} E_r = \sum_{r=0}^{n} p_i(r) E_r.
\]
The scalars $p_i(j)$ are known as the eigenvalues of the scheme.

On the other hand, the matrices $A_0, \ldots, A_n$ are a basis for the algebra and thus there are scalars $q_i(j)$ such that

$$E_j = 2^{-n} \sum_{r=0}^{n} q_j(r) A_r.$$ 

The scalars $q_i(j)$ are the dual eigenvalues of the scheme.

If $f$ is any function defined on the eigenvalues of the scheme then

$$f(A_1) = \sum_{r=0}^{n} f(p_1(r)) E_r.$$ 

For the $n$-cube, $p_1(r) = n - 2r$ and accordingly

$$H(t) = \sum_{r=0}^{n} \exp(i(n-2r)t) E_r = \exp(int) \sum_{r=0}^{n} \exp(-2irt) E_r.$$ 

If we set $t = \pi$, we then have

$$H(\pi) = (-1)^n \sum_{r=0}^{n} E_r = (-1)^n I.$$ 

Thus the $n$-cube is periodic with period $\pi$. Now try $n = \pi/2$. Then

$$H(\pi/2) = i^n \sum_{r=0}^{n} (-1)^r E_r.$$ 

From, for example, [9, Section 21.3] we know that

$$\sum_{r=0}^{n} (-1)^r E_r = A_d$$

and we conclude that perfect state transfer occurs at time $\pi/2$.

In [8], Jafarizadeh and Sufiani give examples of perfect state transfer on distance-regular graphs that arise when a weighted adjacency matrix is used in place of the ordinary adjacency matrix.
9 Hadamard Matrices

We now show how to use a special class of Hadamard matrices to construct distance-regular graphs of diameter three with perfect state transfer.

The Hadamard matrices $H$ we want must be as follows:

(a) Symmetric: $H = H^T$.

(b) Regular: all row and column sums are equal.

(c) Constant diagonal: all entries on the diagonal are equal.

Suppose $H$ is $n \times n$ and satisfies this constellation of conditions. If its rows sum to $c$, then

$$c^2 I = H^2 I = HH^T = nI,$$

whence $c = \pm \sqrt{n}$. It follows that there are two possibilities: either the diagonal entries and the rows sums of $H$ have the same sign, or they do not. To handle this we assign a parameter $\epsilon = \epsilon(H)$ to $H$, by defining $\epsilon$ to be the sign of the product of the row sum of $H$ with a diagonal entry. Whatever the value of $\epsilon(H)$, the order of $H$ must be a square. For a recent useful paper on these Hadamard matrices, see Haemers [7].

We remark that if the row sums of a Hadamard matrix are all equal then its columns sums must all be equal as well, and again the order of the matrix must be a square. Similarly, a symmetric Hadamard matrix with constant diagonal must have square order. If $H$ and $K$ are regular symmetric Hadamard matrices with constant diagonal, then so is their Kronecker product $H \otimes K$ and

$$\epsilon(H \otimes K) = \epsilon(H)\epsilon(K).$$

Finally if $H$ is a regular Hadamard matrix of order $n \times n$ with constant diagonal, and $P$ is the permutation matrix on $\mathbb{R}^n \otimes \mathbb{R}^n$ defined by

$$P(u \otimes v) = v \otimes u,$$

then $P(H \otimes H^T)$ is a symmetric regular Hadamard matrix with constant diagonal.

Suppose $H$ is a regular symmetric $n \times n$ Hadamard matrix with constant diagonal. Replacing $H$ by $-H$ is necessary, we may assume that the diagonal entries of $H$ are equal to 1, and then the matrix

$$\frac{1}{2}(J + H) - I$$

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is the adjacency matrix of a regular graph (in fact a strongly regular graph). Unfortunately the graphs that result are not the ones we need. Our aim rather is to construct an antipodal distance-regular graph of diameter three on \(2n\) vertices from \(H\). (These graphs are member of a class known as *regular two-graphs*. An introductory treatment is offered in [6, Chapter 11])

We construct our graphs as follows. Let \(H\) be a symmetric Hadamard matrix of order \(n \times n\) with constant row sum and with all diagonal entries equal to 1. We construct a graph \(X(H)\) with vertex set

\[
\{1, \ldots, n\} \times \{0, 1\},
\]

where \((i, a)\) is adjacent to \((j, b)\) if and only if \(i \neq j\) and

\[
H_{i,j} = (-1)^{a+b}
\]

Clearly this gives us a regular graph \(X(H)\) on \(2n\) vertices with valency \(n - 1\). It is not hard to check that its diameter is three, and two vertices are at distance three if and only if they are of the form

\[(i, 0), (i, 1)\]

for some \(i\). Suppose \(A\) is the adjacency matrix of \(X(H)\). The space \(S\) of vectors that are constant on the antipodal classes of \(X(H)\) has dimension \(n\) and the matrix representing the action of \(A\) on \(S\) is the \(n \times n\) matrix \(J_1\). Its eigenvalues are \(n - 1\) and \(-1\) with respective multiplicities \(1\) and \(n - 1\). The orthogonal complement of \(S\) is also \(A\)-invariant and the matrix representing the action of \(A\) is \(H\).

If we write \(H\) as \(I + C - D\) where \(C\) and \(D\) are 01-matrices, then

\[
A(X(H)) = C \otimes \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + D \otimes \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}
\]

and the eigenvalues of \(A\) are the eigenvalues of the matrices

\[
C + D = J - I, \quad C - D = H - I.
\]

Therefore the eigenvalues of \(A\) are \(n - 1\), \(-1\) and the eigenvalues of \(H - I\). Since \(H^2 = nI\), we see that the eigenvalues of \(A\) are

\[
n - 1, -1, \sqrt{n} - 1, -\sqrt{n} - 1.
\]
If $a$ is the multiplicity of $\sqrt{n}$ as an eigenvalue of $F$, then

$$n = \text{tr}(A) = a\sqrt{n} - (n - a)\sqrt{n}$$

whence

$$a = \frac{1}{2}(n + \sqrt{n}).$$

it follows that

$$\mu(z) = z^{n-1} + (n - 1)z^{-1} + \frac{1}{2}(n + \sqrt{n})z^{\sqrt{n}-1} + \frac{1}{2}(n - \sqrt{n})z^{-\sqrt{n}-1}$$

$$= z^{-\sqrt{n}-1}(z^{n+\sqrt{n}} + (n - 1)z^{\sqrt{n}} + \frac{1}{2}(n - \sqrt{n})z^{2\sqrt{n}} + \frac{1}{2}(n - \sqrt{n})).$$

If $z\sqrt{n} = -1$, then $z^2\sqrt{n} = 1$ and, since $\sqrt{n}$ is even,

$$z^{n-\sqrt{n}} = (z^{\sqrt{n}})^{\sqrt{n}}z^{-\sqrt{n}} = -1.$$ 

Therefore if $z\sqrt{n} = -1$, then $\mu(z) = 0$ and if $z = e^{it}$ then

$$H(t) = -E_{n-1} - E_{(-1)} + E_{(-1+\sqrt{n})} + E_{(-1-\sqrt{n})}.$$ 

Let $F$ be the direct sum of $n$ copies of the matrix

$$\frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$ 

Then $\text{rk}(F) = n$ and $\text{col}(F)$ is the space of functions constant on the antipodal classes of $X(H)$. Since $F^2 = F$, we find that $E_{(-1)} = F - E_{n-1}$ and consequently

$$H(t) = I - 2F.$$ 

So $H(t)$ is a permutation matrix and we have perfect state transfer.

Infinitely many examples of regular symmetric Hadamard matrices with constant diagonal are known, in particular they exist whenever the order $n$ is a power of four. Haemers [7] provides a recent summary of the state of our knowledge.
10 Questions and Comments

We mention some problems raised by our work.

(a) Are there periodic graphs on an even number of vertices which do not have integer eigenvalues?

(b) Is there an example where perfect state transfer occurs and the underlying graph is not periodic? (Such a graph could not be regular.)

(c) In all examples where we have perfect state transfer in a graph $X$, the vertices involved are at maximum distance in $X$. Must this be true in all cases?

Facer, Twamley and Cresser [4] construct certain Cayley graphs for $\mathbb{Z}_2^d$ on which perfect state transfer; the resulting family of graphs include the $n$-cubes. It seems that there is some chance we might be able to characterize the Cayley graphs for $\mathbb{Z}_2^d$ where perfect state transfer occurs.

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