Linear Algebra and its Applications 531 (2017) 516–532

Contents lists available at ScienceDirect

Linear Algebra and its Applications

www.elsevier.com/locate/laa

Universality in perfect state transfer

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A R T I C L E I N F O

Article history:
Received 18 January 2017
Accepted 11 June 2017
Available online 15 June 2017
Submitted by R. Brualdi

MSC:
05C50

Keywords:
Quantum walk
Perfect state transfer
Circulant
Cyclotomic fields

A B S T R A C T

A continuous-time quantum walk on a graph is a matrix-valued function $\exp(-\mathrm{i}At)$ over the reals, where A is the adjacency matrix of the graph. Such a quantum walk has universal perfect state transfer if for all vertices u, v, there is a time where the (v, u) entry of the matrix exponential has unit magnitude. We prove new characterizations of graphs with universal perfect state transfer. This extends results of Cameron et al. (2014) [3]. Also, we construct non-circulant families of graphs with universal perfect state transfer. All prior known constructions were circulants. Moreover, we prove that if a circulant, whose order is prime, prime squared, or a power of two, has universal perfect state transfer then its underlying graph must be complete. This is nearly tight since there are universal perfect state transfer circulants with non-prime-power order where some edges are missing.

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http://dx.doi.org/10.1016/j.laa.2017.06.015

1. Introduction

A *continuous-time quantum walk* on a graph is given by the one-parameter matrix-valued map $U(t) = \exp(-\mathtt{i}At)$, where A is the adjacency matrix of the graph. This notion was introduced by Farhi and Guttman [6] to study quantum algorithms for search problems. Using this formulation, Bose [2] studied problems related to information transmission in quantum spin chains. In such a quantum walk, we say that there is *perfect state transfer* from vertex u to vertex v at time τ if the (v, u) entry of $U(\tau)$ has unit magnitude.

Kay [13] showed that if a graph, whose adjacency matrix is real symmetric, has perfect state transfer from u to v and also from u to w, then v must be equal to w. Cameron et al. [3] showed that it is possible to violate this "monogamy" property in graphs whose adjacency matrices are complex Hermitian matrices. They studied graphs with a *universal* property where perfect state transfer occurs between every pair of vertices. The smallest nontrivial example is the circulant graph $\mathtt{Circ}(0, -\mathtt{i}, \mathtt{i})$, whose adjacency matrix is

$$\begin{bmatrix} 0 & -\mathtt{i} & \mathtt{i} \\ \mathtt{i} & 0 & -\mathtt{i} \\ -\mathtt{i} & \mathtt{i} & 0 \end{bmatrix}. \tag{1}$$

Some work related to universality in state transfer for quantum computing applications may be found in [14].

We may view certain graphs whose adjacency matrices are Hermitian matrices as *gain* graphs. These are graphs whose "directed" edges are labeled with elements from a group Γ. If the edge (u, v) is labeled with group element $g \in \Gamma$, then the reversed edge (v, u) is labeled with g^{-1}. If Γ is the circle group, we get the so-called complex unit gain graphs (see Reff [16]). In our case, we simply require that edges in opposite directions have weights which are complex conjugates to each other.

Our main goal is to characterize graphs with universal perfect state transfer. Cameron et al. [3] proved strong necessary conditions for graphs with the universal perfect state transfer property. They showed that such graphs must have distinct eigenvalues, their unitary diagonalizing matrices must be type-II (see Chan and Godsil [4]), and their switching automorphism group must be cyclic. A spectral characterization for circulants with the universal property was also proved in [3].

In this work, we extend some of the observations from Cameron et al. [3]. More specifically, we prove new characterizations of graphs with universal perfect state transfer. The first characterization exploits the fact that the unitary diagonalizing matrix of the graph admits a canonical form. This allows us to show a tight connection between the spectra of the graph with the perfect state transfer times. Our second characterization is on circulants with the universal property. It involves the set of minimum times when perfect state transfer occur between pairs of vertices. If universal perfect state transfer occurs, then the quantum walk starting at any vertex will exhibit perfect state transfer to all other vertices before returning to the starting vertex. We consider the time intervals between these perfect state transfers to the other (non-starting) vertices. We prove that these time intervals are equally spaced (they have the same lengths) if and only if the underlying graph with universal perfect state transfer is circulant. This complements the observation in [3] which characterizes the switching automorphism group of circulants with the universal property.

Most of the examples studied in [3] were circulants whose nonzero weights are $\pm\mathtt{i}$. Here, we provide a construction of *non-circulant* graphs of composite order with the universal property. To the best of our knowledge, this is the first known example of such family of graphs. We show that these families are non-circulant by appealing to our second characterization above (based on spacings of the minimum perfect state transfer times).

Finally, we provide a nearly tight characterization of circulants with the universal property in terms of the number of nonzero coefficients. We show that if a circulant has universal perfect state transfer and its order is prime, square of a prime, or a power of two, then all of its off-diagonal coefficients must be nonzero. As a partial converse, we show an infinite family of circulants with universal perfect state transfer whose order is not a prime power and where some off-diagonal coefficients are zero.

We conclude by studying universal perfect state transfer in complex unit gain graphs. The only known examples of complex unit gain graphs with the universal property are the circulants K_2 and $\mathtt{Circ}(0, -\mathtt{i}, \mathtt{i})$. We conjecture that this set is unique.

For a recent survey and a comprehensive treatment of quantum walk on graphs, we refer the interested reader to Godsil [8,7].

2. Preliminaries

A weighted graph $G = (V, E, w)$ is defined by a vertex set V, an edge set E and a weight function $w : E \to \mathbb{C}$. If G has n vertices, we will often identify the vertex set with $\mathbb{Z}/n\mathbb{Z}$. The adjacency matrix $A(G)$ of graph G is a $n \times n$ matrix defined as $A(G)_{k,j} = w(j, k)$ if $(j, k) \in E$, and $A(G)_{k,j} = 0$ otherwise. For a vertex u, we use $\mathbf{e}_u$ to denote the characteristic vector of u. A graph is Hermitian if its adjacency matrix is (see [11]).

For complex numbers $a_0, \ldots, a_{n-1} \in \mathbb{C}$, we let $C = \mathtt{Circ}(a_0, \ldots, a_{n-1})$ denote the circulant matrix of order n where $C_{jk} = a_{k-j}$, for $j, k \in \mathbb{Z}/n\mathbb{Z}$. If C is Hermitian, note that a_0 must be real and $a_{n-j} = \overline{a}_j$, for $j = 1, \ldots, n-1$. It is known that any circulant is diagonalized by the Fourier matrix F_n defined by $(F_n)_{jk} = \zeta_n^{jk}/\sqrt{n}$. Here, $\zeta_n = e^{2\pi\mathtt{i}/n}$ denotes a primitive nth root of unity.

We call a matrix *flat* if all of its entries have the same magnitude. A unitary matrix is type-II if and only if it is flat (see Chan and Godsil [4]). Note that the Fourier matrix is type-II. A *monomial* matrix is a product of a permutation matrix and an invertible diagonal matrix (see Davis [5]). Two matrices A and B are *switching equivalent* if $MA = BM$ for some monomial matrix. The *switching automorphism group* of a graph G, denoted $\texttt{SwAut}(G)$, is the group of all monomial matrices which commute with $A(G)$. This generalizes the notion of an automorphism group of a graph.

For more background on algebraic graph theory, see Godsil and Royle [12].

3. Basic properties

The following result shows strong necessary conditions for graphs with universal perfect state transfer.

Theorem 1. *(Cameron et al. [3]) Let G be a Hermitian graph with universal perfect state transfer. Then, the following hold:*

1. *All eigenvalues of G are distinct.*
2. *The adjacency matrix of G is unitarily diagonalized by a flat matrix.*
3. *The switching automorphism group of G is cyclic whose order divides the size of G.*

We show some additional properties of graphs with universal perfect state transfer.

Definition 1. Let G be a graph with universal perfect state transfer. For every pair of vertices v and w of G, we let $T_{v,w}$ denote the set of times where perfect state transfer occurs from v to w. That is,

$$T_{v,w} := \{t \in \mathbb{R}^+ : |\langle \mathbf{e}_w, e^{-\mathrm{i}A(G)t}\mathbf{e}_v\rangle| = 1\}. \tag{2}$$

Fact 1. Let G be a graph with universal perfect state transfer. For each pair of vertices v and w, $T_{v,w}$ is a discrete additive subgroup of $\mathbb{R}$.

Proof. See Godsil [7] or Cameron et al. [3]. □

Since $T_{v,w}$ is a discrete additive subgroup of the reals, it has a smallest element. We will denote the minimum element of the above set as $t_{v,w} := \min T_{v,w}$.

Lemma 1. *Let G be a graph with universal perfect state transfer and let u be a vertex of G. Then, for all vertices $v \neq u$, we have $t_{u,v} < t_{u,u}$.*

Proof. If $t_{u,v} > t_{u,u}$, let q be the largest integer for which $qt_{u,u} < t_{u,v}$. Then, $\hat{t} = t_{u,v} - qt_{u,u}$ is an element of $T_{u,v}$ which is smaller than $t_{u,v}$. □

Lemma 2. *Let G be a graph and let u be an arbitrary vertex of G. Then G has universal perfect state transfer if and only if perfect state transfer occurs from u to all vertices of G.*

Proof. It suffices to prove only one direction since the other direction is immediate. Suppose that perfect state transfer occurs from u to all vertices. By Lemma 1, the quantum walk starting at u *visits* all the other vertices before returning to u. If $t_{u,v} < t_{u,w}$ then perfect state transfer occurs from v to w. But, there is also perfect state transfer from w to v since the quantum walk has perfect state transfer from w back to u (at time $t_{u,u} - t_{u,w}$) and then from u to v (at time $t_{u,v}$). This proves that there is perfect state transfer between every pair of vertices. □

4. Canonical flatness

A flat unitary matrix is also called a *type-II* matrix (see [4]). We say that a type-II matrix is in *canonical* form if both its first row and its first column are the all-one vector.

Lemma 3. *Let G be a Hermitian graph on n vertices with universal perfect state transfer. Then G is unitarily diagonalized by a type-II matrix X in canonical form:*

$$X = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 & 1 & 1 & \dots & 1 \\ 1 & e^{\mathbf{i}\alpha_{1,1}} & e^{\mathbf{i}\alpha_{1,2}} & \dots & e^{\mathbf{i}\alpha_{1,n-1}} \\ 1 & e^{\mathbf{i}\alpha_{2,1}} & e^{\mathbf{i}\alpha_{2,2}} & \dots & e^{\mathbf{i}\alpha_{2,n-1}} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & e^{\mathbf{i}\alpha_{n-1,1}} & e^{\mathbf{i}\alpha_{n-1,2}} & \dots & e^{\mathbf{i}\alpha_{n-1,n-1}} \end{bmatrix} \tag{3}$$

where $\alpha_{j,k} \in [0, 2\pi)$.

Proof. Suppose A is the Hermitian adjacency matrix of G that is unitarily diagonalized by Z. Then, $AZ = Z\Lambda$ where Λ is a diagonal matrix of the eigenvalues of A. The columns of Z are the eigenvectors of A which we will denote as $z_0, \dots, z_{n-1}$. Let D be a diagonal matrix defined as $D_{jj} = 1/\langle \mathbf{e}_0, z_j \rangle$. Then, $\tilde{Z} = ZD$ is also a flat unitary which diagonalizes A but with $\langle \mathbf{e}_0, \tilde{z}_k \rangle = 1$, for each $k = 0, \dots, n-1$. Next, consider a diagonal switching matrix S defined as $S_{jj} = 1/\langle \mathbf{e}_j, \tilde{z}_0 \rangle$. Then, we have

$$\tilde{A} = (S\tilde{Z})\Lambda(S\tilde{Z})^{-1}. \tag{4}$$

Note $\tilde{A} = SAS^{-1}$ is switching equivalent to A. Since $X = S\tilde{Z}$ is a flat unitary matrix of the claimed form, we are done. □

Corollary 1. *Let M be a flat unitary matrix in canonical form. Then, except for the first row and the first column, the row sums and the column sums of M are zero.*

Proof. Since the columns are orthonormal and the first column is the all-one vector, it is clear that the column sums must be zero. The row sums are zero since M^T is unitary whenever M is. □

Using Lemma 3, we show a spectral characterization of graphs with universal perfect state transfer.

Theorem 2. *Let G be a n-vertex Hermitian graph with eigenvalues $\lambda_0, \dots, \lambda_{n-1}$. Suppose G is diagonalized by a canonical type-II matrix X, where $X_{j,k} = e^{\mathrm{i}\alpha_{j,k}}/\sqrt{n}$ with $\alpha_{j,k} \in [0, 2\pi)$ and $\alpha_{j,k} = 0$ if either j or k is zero. Then, G has universal perfect state transfer if and only if for each $\ell = 0, \dots, n-1$, there is $t_\ell \in \mathbb{R}$ so that for all $k = 1, \dots, n-1$, we have*

$$(\lambda_k - \lambda_0)t_\ell = \alpha_{\ell,k}. \tag{5}$$

Proof. Let A be the Hermitian adjacency matrix of G. We denote the kth column of X as z_k which is the eigenvector of A corresponding to eigenvalue λ_k. Thus,

$$e^{-\mathrm{i}At} = \sum_{k=0}^{n-1} e^{-\mathrm{i}\lambda_k t} z_k z_k^\dagger. \tag{6}$$

($\Rightarrow$) Assume G has universal perfect state transfer. Suppose that perfect state transfer from vertex 0 to vertex ℓ occurs at time $t_\ell \in \mathbb{R}$ with phase $e^{\mathrm{i}\theta_\ell}$. Then,

$$\langle \mathbf{e}_\ell, e^{-\mathrm{i}At_\ell}\mathbf{e}_0\rangle = \sum_{k=0}^{n-1} e^{-\mathrm{i}\lambda_k t_\ell}\langle \mathbf{e}_\ell, z_k\rangle\langle z_k, \mathbf{e}_0\rangle = \frac{1}{n}\sum_{k=0}^{n-1} e^{-\mathrm{i}\lambda_k t_\ell} e^{\mathrm{i}\alpha_{\ell,k}}. \tag{7}$$

Moreover, we have

$$e^{\mathrm{i}\theta_\ell} = \frac{1}{n}\left[e^{-\mathrm{i}\lambda_0 t_\ell} + \sum_{k=1}^{n-1} e^{-\mathrm{i}(\lambda_k t_\ell - \alpha_{\ell,k})}\right]. \tag{8}$$

So, for each $k = 1, \dots, n-1$, we have $\lambda_k t_\ell - \alpha_{\ell,k} = \lambda_0 t_\ell$, which shows these conditions are necessary for universal perfect state transfer.

($\Leftarrow$) Suppose that for each ℓ, there is a time t_ℓ so that for each $k \neq 0$,

$$(\lambda_k - \lambda_0)t_\ell = \alpha_{\ell,k}. \tag{9}$$

Then,

$$\langle \mathbf{e}_\ell, e^{-\mathrm{i}At_\ell}\mathbf{e}_0\rangle = \frac{1}{n}\sum_{k=0}^{n-1} e^{-\mathrm{i}\lambda_k t_\ell} e^{\mathrm{i}\alpha_{\ell,k}} = e^{-\mathrm{i}\lambda_0 t_\ell}. \tag{10}$$

This shows that there is perfect state transfer from 0 to ℓ. Therefore, there is perfect state transfer from 0 to all vertices. By Lemma 2, this shows there is perfect state transfer between every pair of vertices. □

5. Circulants revisited

Cameron et al. [3] showed the following result on the switching automorphism group of circulants with universal perfect state transfer.

Theorem 3. *(Cameron et al. [3]) Let G be a graph with universal perfect state transfer. Then, G is switching isomorphic to a circulant if and only if* $\texttt{SwAut}(G)$ *is cyclic of order n.*

In what follows, we provide new characterizations of circulants with universal perfect state transfer. The first one is based on the set of times when perfect state transfer occur. The second one is based on the explicit form of allowable weights.

Recall that $T_{u,v}$ is the set of times (positive real numbers) when perfect state transfer occur from vertex u to vertex v. Also, we denote $t_{u,v}$ as the smallest element of $T_{u,v}$.

Theorem 4. *Let G be a n-vertex graph with universal perfect state transfer. Assume that $t_{0,k} < t_{0,k+1}$ for all $k = 1, \ldots, n-2$ and that $t_{0,1} = \min\{t_{k,k+1} : k \in \mathbb{Z}/n\mathbb{Z}\}$. Then, G is switching isomorphic to a circulant if and only if*

$$t_{k,k+1} = t_{0,1}, \tag{11}$$

for all $k \in \mathbb{Z}/n\mathbb{Z}$.

Proof. Let A be the adjacency matrix of G.

($\Rightarrow$) Suppose that G is switching isomorphic to a circulant. Consider the set of times when perfect state transfer occur in G:

$$T = \{t \in \mathbb{R}^+ : \exists j, k \in \mathbb{Z}/n\mathbb{Z},\ |(e^{-\mathtt{i}At})_{k,j}| = 1\}. \tag{12}$$

Since T is a discrete additive subgroup of $\mathbb{R}$, it has a minimum. Without loss of generality, assume that $t_{0,1} = \min T$. Thus,

$$\langle \mathbf{e}_1, e^{-\mathtt{i}At_{0,1}}\mathbf{e}_0\rangle = \gamma, \tag{13}$$

for some $\gamma \in \mathbb{T}$. By Theorem 3, $\texttt{SwAut}(G)$ is cyclic of order n. We may assume that $\tilde{P} = P_\phi D$ generates $\texttt{SwAut}(G)$ where $\phi = (0\ 1\ \ldots\ n-1)$ and D is a diagonal switching matrix. Since $\tilde{P}$ is a switching automorphism, $\tilde{P}^{-1}A\tilde{P} = A$, which implies $e^{-\mathtt{i}At} = \tilde{P}^{-1}e^{-\mathtt{i}At}\tilde{P}$. Therefore,

$$\langle \mathbf{e}_2, e^{-\mathtt{i}At_{0,1}}\mathbf{e}_1\rangle = \tilde{\gamma}\langle \mathbf{e}_1, \tilde{P}^{-1}e^{-\mathtt{i}At_{0,1}}\tilde{P}\mathbf{e}_0\rangle = \tilde{\gamma}\langle \mathbf{e}_1, e^{-\mathtt{i}At_{0,1}}\mathbf{e}_0\rangle, \tag{14}$$

for some $\tilde{\gamma} \in \mathbb{T}$. So, perfect state transfer occurs from 1 to 2 at time $t_{0,1}$. By repeatedly using the same argument, we see that perfect state transfer occurs from k to $k+1$ at time $t_{0,1}$, for $k = 0, 1, \ldots, n-2$.

($\Leftarrow$) Suppose $t_{k,k+1} = t_{0,1}$, for $k \in \mathbb{Z}/n\mathbb{Z}$. This implies that at time $t_{0,1}$ perfect state transfer occurs from k to $k+1$ (simultaneously) from k to $k+1$ for each $k \in \mathbb{Z}/n\mathbb{Z}$. So, assume

$$\langle \mathbf{e}_{k+1}, e^{-\mathrm{i}At_{0,1}} \mathbf{e}_k \rangle = \gamma_k, \tag{15}$$

for some complex unit weight $\gamma_k \in \mathbb{T}$. Thus,

$$e^{-\mathrm{i}At_{0,1}} = \begin{bmatrix} 0 & 0 & \dots & 0 & \gamma_{n-1} \\ \gamma_0 & 0 & \dots & 0 & 0 \\ 0 & \gamma_1 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & \gamma_{n-2} & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & \dots & 0 & 1 \\ 1 & 0 & \dots & 0 & 0 \\ 0 & 1 & \dots & 0 & 0 \\ \vdots & \vdots & \dots & \vdots & \vdots \\ 0 & 0 & \dots & 1 & 0 \end{bmatrix} \begin{bmatrix} \gamma_0 & 0 & \dots & 0 \\ 0 & \gamma_1 & \dots & 0 \\ 0 & 0 & \dots & 0 \\ \vdots & \vdots & \dots & \vdots \\ 0 & 0 & \dots & \gamma_{n-1} \end{bmatrix}, \tag{16}$$

which shows that $e^{-\mathrm{i}At_{0,1}}$ is a monomial matrix. Since it commutes with A, it is a switching automorphism of G. Moreover, it generates $\texttt{SwAut}(G)$. Thus, by Theorem 3, G is switching isomorphic to a circulant. □

Next we find explicit forms for the weights on circulants which have universal perfect state transfer. But, first we state a spectral characterization of circulants with universal perfect state transfer proved by Cameron et al. [3].

Theorem 5. *(Cameron et al. [3]) Let G be a graph that is switching equivalent to a circulant. Then G has universal perfect state transfer if and only if for some integer q coprime with n, for real numbers α, β with $\beta > 0$, the eigenvalues of G are given by*

$$\lambda_k = \alpha + \beta(qk + c_k n), \qquad k = 0, 1, \dots, n-1, \tag{17}$$

where c_k are integers.

Let A be the adjacency matrix of G. In Theorem 5, we may assume $\alpha = 0$ by allowing a diagonal shift $A + \alpha\mathbb{I}$, which does not affect the quantum walk. Furthermore, we may assume $\beta = 1$ by allowing the time scaling $\frac{1}{\beta}A$, which does not affect perfect state transfer. Finally, we may multiply the adjacency matrix with the multiplicative inverse of q modulo n (to cancel the factor q in qk). In summary, we have the following.

Corollary 2. *Let G be a graph that is switching equivalent to a circulant. Then G has universal perfect state transfer if and only if the eigenvalues of G are given by*

$$\lambda_k = k + c_k n, \qquad k = 0, 1, \dots, n-1 \tag{18}$$

where c_k are integers.

Next, we show a general form for the coefficients of a circulant which has universal perfect state transfer.

Theorem 6. *Let* $\texttt{Circ}(a_0, \dots, a_{n-1})$ *be a circulant with universal perfect state transfer. Then, we have*

$$a_j = \frac{1}{\zeta_n^{-j} - 1} + \sum_{k=0}^{n-1} c_k \zeta_n^{-jk}, \qquad j = 1, \dots, n-1 \tag{19}$$

for integers c_k*, where* $k = 0, \dots, n-1$.

Proof. Let $G = \texttt{Circ}(a_0, \dots, a_{n-1})$. By Corollary 2, the eigenvalues of G are of the form $\lambda_k = k + c_k n$, for some integers c_k, where $k \in \mathbb{Z}/n\mathbb{Z}$. Since circulants are diagonalized by the Fourier matrix (see Biggs [1], page 16), the coefficients of G are given by

$$a_j = \frac{1}{n} \sum_{k=0}^{n-1} \lambda_k \zeta_n^{-jk}, \qquad j = 1, \dots, n-1. \tag{20}$$

Using the assumed form of λ_k, we get

$$a_j = \frac{1}{n} \sum_{k=0}^{n-1} (k + c_k n) \zeta_n^{-jk} = \frac{1}{n} \sum_{k=0}^{n-1} k \zeta_n^{-jk} + \sum_{k=0}^{n-1} c_k \zeta_n^{-jk}. \tag{21}$$

Let $U = \sum_{k=0}^{n-1} k \zeta_n^{-jk}$ and $L = \sum_{k=1}^{n-2} \sum_{\ell=1}^{k} \zeta_n^{-j\ell}$. Note that

$$L + U = (n-1) \sum_{k=1}^{n-1} \zeta_n^{-jk} = 1 - n. \tag{22}$$

Now, we have

$$L = \sum_{k=1}^{n-2} \sum_{\ell=1}^{k} \zeta_n^{-j\ell} = \sum_{k=1}^{n-2} \left(\frac{\zeta_n^{-j(k+1)}}{\zeta_n^{-j} - 1} - 1 \right) \tag{23}$$

$$= \frac{1}{\zeta_n^{-j} - 1} \left(\sum_{k=2}^{n-1} \zeta_n^{-jk} - (n-2) \zeta_n^{-j} \right) \tag{24}$$

$$= 1 - n - \frac{n}{\zeta_n^{-j} - 1}. \tag{25}$$

Thus, $U = n/(\zeta_n^{-j} - 1)$. Therefore,

$$a_j = \frac{1}{\zeta_n^{-j} - 1} + \sum_{k=0}^{n-1} c_k \zeta_n^{-jk}. \quad \square \tag{26}$$

6. Non-circulants with universal state transfer

In this section, we show a construction of a family of non-circulant graphs with universal perfect state transfer. This provides the first known examples of non-circulant families with universal perfect state transfer.

Theorem 7. *Let $n = ab$ be an integer where $a \geq b \geq 2$ are integers. Fix an integer $\beta \geq 2$ and for a positive integer d, let ϑ_d be a function which maps elements of $\mathbb{Z}/n\mathbb{Z}$ to the positive integers defined as*

$$\vartheta_d(x) := \beta\lfloor x/d \rfloor d + x \bmod d. \tag{27}$$

Let X be a $n \times n$ matrix whose (j, k)-entry is given by

$$X_{j,k} = \frac{1}{\sqrt{n}} \zeta_{\beta n}^{\vartheta_a(j)\vartheta_b(k)}. \tag{28}$$

Then, X is type-II. Moreover, if G is the graph with eigenvalues $\{\vartheta_b(k) : k = 0, 1, \ldots, n-1\}$ whose adjacency matrix is unitarily diagonalized by X, then G has universal perfect state transfer.

Proof. First, we show that X is type-II. It is clear that X is flat from its definition. So, it suffices to show that the columns of X form an orthonormal set. In what follows, for $k, \ell \in \mathbb{Z}/n\mathbb{Z}$, let $Q_b(k, \ell) = \lfloor k/b \rfloor - \lfloor \ell/b \rfloor$ and $R_b(k, \ell) = k \bmod b - \ell \bmod b$. If X_k and X_ℓ are the kth and ℓth columns of X, then

$$\langle X_\ell, X_k \rangle = \frac{1}{n} \sum_{j=0}^{n-1} \zeta_{\beta n}^{M_b(k,\ell)\vartheta_a(j)}, \quad \text{where } M_b(k,\ell) = \beta Q_b(k,\ell) b + R_b(k,\ell) \tag{29}$$

$$= \frac{1}{n} \sum_{r=0}^{a-1} \zeta_{\beta n}^{M_b(k,\ell) r} \sum_{q=0}^{b-1} \left(\zeta_n^{a M_b(k,\ell)}\right)^q. \tag{30}$$

But, note that for any integer $M \neq 0$, provided $\zeta_b^M \neq 1$, we have

$$\sum_{q=0}^{b-1} (\zeta_n^{aM})^q = \frac{\zeta_n^{abM} - 1}{\zeta_n^{aM} - 1} = 0, \tag{31}$$

since $\zeta_n^{ab} = 1$. So, if $R_b(k, \ell) \neq 0$, then $M_b(k, \ell) \neq 0$, which implies $\langle X_\ell, X_k \rangle = 0$. On the other hand, if $R_b(k, \ell) = 0$, then $Q_b(k, \ell) \neq 0$, for otherwise $k = \ell$. Here, we have

$$\langle X_\ell, X_k \rangle = \frac{1}{n} \sum_{q=0}^{b-1} \zeta^{q\beta Q_b(k,\ell)} \sum_{r=0}^{a-1} \left(\zeta_a^{Q_b(k,\ell)}\right)^r \tag{32}$$

Thus, $\langle X_\ell, X_k \rangle = 0$ also holds.

Next, we show that G has universal perfect state transfer. If we let

$$\alpha_{j,k} = \frac{2\pi}{\beta n}\vartheta_a(j)\vartheta_b(k), \tag{33}$$

for $j, k \in \mathbb{Z}/n\mathbb{Z}$, then $X_{j,k} = e^{\mathrm{i}\alpha_{j,k}}$. For each $j \in \mathbb{Z}/n\mathbb{Z}$, let $t_j = (2\pi/\beta n)\vartheta_a(j)$. Then,

$$\lambda_k t_j = \alpha_{j,k} \tag{34}$$

holds for all $k \in \mathbb{Z}/n\mathbb{Z}$, since $\lambda_k = \vartheta_b(k)$ and $\lambda_0 = 0$. By Theorem 2, this shows that G has universal perfect state transfer.

Finally, we show that G is not switching equivalent to a circulant. By Theorem 4, it suffices to show that $t_{j+1} - t_j$ are not all equal. From the definition of $\vartheta_a(j)$, we have $t_1 - t_0 = \frac{2\pi}{\beta n}$ whereas $t_a - t_{a-1} = \frac{2\pi}{\beta n}((\beta - 1)a + 1)$. □

Example 1. For $k \geq 2$, let G_k be a graph of order 4 with eigenvalues $\{0, 1, 2k, 2k+1\}$. In Theorem 7, we let $\beta = k$, $a = b = 2$ (and $n = 4$). Let X be the following unitary matrix (whose columns are the eigenvectors of G_k):

$$X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & e^{\mathrm{i}\pi/2k} & e^{\mathrm{i}\pi} & e^{\mathrm{i}\pi(2k+1)/2k} \\ 1 & e^{\mathrm{i}\pi} & e^{2\pi\mathrm{i}} & e^{\mathrm{i}\pi} \\ 1 & e^{\mathrm{i}\pi(2k+1)/2k} & e^{\mathrm{i}\pi} & e^{\mathrm{i}\pi/2k} \end{bmatrix} \tag{35}$$

Let $A = X\Lambda X^{-1}$, where $\Lambda = \mathrm{diag}(0, 1, 2k, 2k+1)$ be the adjacency matrix of G_k. By Theorem 7, G_k has universal perfect state transfer.

Note G_3 is a non-circulant graph with universal perfect state transfer. The eigenvalues of G_3 are $\{0, 1, 6, 7\}$ and its adjacency matrix is

$$A = \begin{bmatrix} 0 & \frac{3}{2}(1 + e^{-\mathrm{i}\pi/6}) & \frac{1}{2} & \frac{3}{2}(1 - e^{-\mathrm{i}\pi/6}) \\ \frac{3}{2}(1 + e^{\mathrm{i}\pi/6}) & 0 & \frac{3}{2}(1 - e^{\mathrm{i}\pi/6}) & \frac{1}{2} \\ \frac{1}{2} & \frac{3}{2}(1 - e^{-\mathrm{i}\pi/6}) & 0 & \frac{3}{2}(1 + e^{-\mathrm{i}\pi/6}) \\ \frac{3}{2}(1 - e^{\mathrm{i}\pi/6}) & \frac{1}{2} & \frac{3}{2}(1 + e^{\mathrm{i}\pi/6}) & 0 \end{bmatrix}. \tag{36}$$

7. Denseness

In this section, we show that if a circulant has universal perfect state transfer, then all of its coefficients must be nonzero under certain conditions on the order.

Definition 2. A circulant $\mathtt{Circ}(a_0, a_1, \ldots, a_{n-1})$ is called *dense* if $a_j \neq 0$ for $j = 1, \ldots, n-1$.

Our main result in this section is the following.

Theorem 8. *Let $G = \mathtt{Circ}(a_0, \ldots, a_{n-1})$ be a circulant with universal perfect state transfer. If n is a prime, square of a prime, or a power of two, then G is dense.*

We will divide the proof of the theorem into several lemmas. First, we consider the case when the order of the circulant is prime.

Lemma 4. *For a prime p, let* $\texttt{Circ}(a_0, \ldots, a_{p-1})$ *be a circulant with universal perfect state transfer. Then,* $a_j \neq 0$ *for* $j = 1, \ldots, p-1$.

Proof. We may assume that $\lambda_0 = 0$ (by a diagonal shift). Since $a_j = \frac{1}{p}\sum_{k=1}^{p-1} \lambda_k \zeta_p^{-jk}$, we have that $a_j \in \mathbb{Q}(\zeta_p)$. Note that $\{\zeta_p^j : j = 1, \ldots, p-1\}$ is a basis for the cyclotomic field extension $\mathbb{Q}(\zeta_p)/\mathbb{Q}$. Thus, if $a_j = 0$ for some $j \neq 0$, then $\lambda_k = 0$ for all $k \neq 0$. But, this is a contradiction to the assumed form of λ_k in (18). □

Second, we consider universal perfect state transfer in circulants whose order is the square of a prime.

Lemma 5. *Given a prime p, let $n = p^2$. For a circulant* $\texttt{Circ}(a_0, \ldots, a_{n-1})$*, suppose* $a_j \in \mathbb{Q}$ *for some* $j \neq 0$. *Then,* $a_d = a_j$ *for* $d = \gcd(j, n)$.

Proof. Let $j \in \{1, \ldots, n-1\}$ and $d = \gcd(j, n)$. Then, there is $\ell \in (\mathbb{Z}/n\mathbb{Z})^\star$ so that $j\ell \equiv d \pmod n$. To see this, note $j\ell \equiv d \pmod n$ is solvable since $\gcd(j, n)$ divides d. Moreover, $\gcd(\ell, n) = 1$ since $\gcd(\ell, n/d) = 1$ and $\gcd(\ell, d) = 1$. Here, we used the fact that $n = p^2$.

Since $\texttt{Gal}(\mathbb{Q}(\zeta_n)/\mathbb{Q}) = (\mathbb{Z}/n\mathbb{Z})^\star$, there is a field automorphism ϕ_ℓ of $\mathbb{Q}(\zeta_n)$ which fixes $\mathbb{Q}$ for which $\phi_\ell(\zeta_n) = \zeta_n^\ell$. Since $a_j = (1/n)\sum_{k=0}^{n-1} \lambda_k \zeta_n^{-jk}$, we have

$$\phi_\ell(a_j) = \frac{1}{n}\sum_{k=0}^{n-1} \lambda_k \zeta_n^{-\ell jk} = \frac{1}{n}\sum_{k=0}^{n-1} \lambda_k \zeta_n^{-dk} = a_d. \tag{37}$$

But, $\phi_\ell(a_j) = a_j$ since $a_j \in \mathbb{Q}$. This shows $a_j = a_d$. □

Lemma 6. *Let* $G = \texttt{Circ}(a_0, \ldots, a_{n-1})$ *be a circulant of order n with universal perfect state transfer. If d is an odd divisor of n and n/d is prime, then* $a_d \neq 0$.

Proof. Let $p = n/d$ be prime. Then,

$$a_d = \frac{1}{n}\sum_{k=0}^{n-1} \lambda_k \zeta_n^{-dk} = \frac{1}{p}\sum_{k=0}^{p-1} \Lambda_k \zeta_p^{-k}, \tag{38}$$

where $\Lambda_k = \frac{1}{d}\sum_{\ell=0}^{d-1} \lambda_{k+\ell p}$. By Corollary 2, we have

$$\Lambda_k = \frac{1}{d}\sum_{\ell=0}^{d-1} (k + \ell p + n\mathbb{Z}) = k + \frac{p(d-1)}{2} + n\mathbb{Z}. \tag{39}$$

Using this in (38) combined with the fact that $\sum_{k=0}^{p-1} \zeta_p^{-k} = 0$, we get

$$a_d = \frac{1}{p} \sum_{k=0}^{p-1} \left(k + \frac{p(d-1)}{2} + n\mathbb{Z} \right) \zeta_p^{-k} \tag{40}$$

$$= \frac{1}{p} \sum_{k=1}^{p-1} k\zeta_p^{-k}. \tag{41}$$

Since ζ_p^k, for $k = 1, \dots, p-1$, are linearly independent, we have $a_d \neq 0$. □

For our next lemma, we will need the following fact about connectivity in circulants.

Fact 2. (Meijer [15], Theorem 4.2) A circulant $\texttt{Circ}(a_0, \dots, a_{n-1})$ is connected if and only if $\gcd(\{j : a_j \neq 0\} \cup \{n\}) = 1$.

Lemma 7. *For a prime p, suppose $n = p^2$. Let $G = \texttt{Circ}(a_0, \dots, a_{n-1})$ be a circulant with universal perfect state transfer. Then, $a_j \neq 0$ for all $j \neq 0$.*

Proof. Suppose $a_j = 0$ for some $j \neq 0$. By Lemma 5, we have $a_d = 0$ for $d = \gcd(j, n)$. Since $n = p^2$, we have two cases to consider: $d = 1$ or $d = p$. If $a_1 = 0$, then G is not connected by Fact 2. If $a_p = 0$, then this contradicts Lemma 6. □

Finally, we consider universal perfect state transfer in circulants whose order is a power of two. Here, we use the following result of Good in a crucial manner.

Fact 3. (Good [10], Theorem 1) If m is a power of two, then $\{e^{i\pi r/m} : r = 0, \dots, m-1\}$ is linearly independent over $\mathbb{Q}$.

Lemma 8. *For a positive integer d, suppose $n = 2^d$. Let $G = \texttt{Circ}(a_0, \dots, a_{n-1})$ be a circulant with universal perfect state transfer. Then, $a_j \neq 0$ for all $j = 1, \dots, n-1$.*

Proof. Given $d \in \mathbb{Z}^+$, let $n = 2^d$ and $m = 2^{d-1}$. Recall that $\zeta_n = e^{2\pi i/n}$. We have

$$a_j = \frac{1}{n} \sum_{k=0}^{n-1} \lambda_k \zeta_n^{-jk} = \frac{1}{2m} \sum_{\ell=0}^{m-1} \Lambda_\ell(j) (e^{i\pi/m})^{-\ell}, \tag{42}$$

where

$$\Lambda_\ell(j) = \sum_{k:jk\equiv\ell} \lambda_k - \sum_{k:jk\equiv m+\ell} \lambda_k \tag{43}$$

By Fact 3, if $a_j = 0$ then $\Lambda_\ell(j) = 0$ for all $\ell = 0, \dots, m-1$. We show that $\Lambda_0 \neq 0$.

We consider the case when $\ell = 0$. If j is odd, then the map $f_j(k) \equiv jk \pmod{n}$ is a bijection. Thus, $\Lambda_0(j) = \lambda_0 - \lambda_m \equiv m \pmod{n}$. Next, suppose j is even with $j = 2^e s$

where $e \geq 1$ and s is odd. Then, the values k for which $jk \equiv 0 \pmod{n}$ are given by $r2^{d-e}$ for $r = 0, 1, \ldots, 2^e - 1$. Also, the values k for which $jk \equiv m \pmod{n}$ are given by $(2r+1)2^{d-e-1}$ for $r = 0, 1, \ldots, 2^e - 1$. Therefore,

$$\Lambda_0 = \sum_{r=0}^{2^e-1} (r2^{d-e} - (2r+1)2^{d-e-1}) \equiv m \pmod{n}. \tag{44}$$

Thus, in both cases we have $\Lambda_0 \not\equiv 0 \pmod{n}$, which implies $\Lambda_0 \neq 0$. □

Proof of Theorem 8. Follows immediately from Lemmas 4, 7, and 8. □

7.1. Non-dense circulants with universal state transfer

We show a partial converse of Theorem 8 by constructing non-dense circulants with universal perfect state transfer whose orders are not prime powers. This observation uses the following fact about cyclotomic units.

Fact 4. (Washington [17], Proposition 2.8) Suppose n is a positive integer which has at least two distinct prime factors. Then $1 - \zeta_n$ is a unit of $\mathbb{Z}[\zeta_n]$. Moreover,

$$\prod_{\substack{0<j<n \\ \gcd(j,n)=1}} (1 - \zeta_n^j) = 1. \tag{45}$$

Note that Fact 4 also implies that $1 - \zeta_n^j$ is a unit of $\mathbb{Z}[\zeta_n]$ for every j with $\gcd(j, n) = 1$.

Proposition 1. *For two distinct primes p and q, let $n = pq$. Let $c_0, \ldots, c_{n-1}$ be integers so*

$$\sum_{k=0}^{n-1} c_k \zeta_n^{-k} = \frac{1}{1 - \zeta_n^{-1}}. \tag{46}$$

Let $a_0 = 0$ and, for $j = 1, \ldots, n-1$, let $a_j = 1/(\zeta_n^{-j} - 1) + \sum_{k=0}^{n-1} c_k \zeta_n^{-jk}$. Then, $G = \texttt{Circ}(a_0, \ldots, a_{n-1})$ is a non-dense circulant with universal perfect state transfer.

Proof. By the choice of the integers c_k in (46), $a_1 = a_{n-1} = 0$. This shows that G is not dense. Also, note that

$$\lambda_0 = \sum_{j=0}^{n-1} a_j = \sum_{j=1}^{n-1} \frac{1}{\zeta_n^{-j} - 1} - \sum_{k=0}^{n-1} c_k. \tag{47}$$

The other eigenvalues are given by $\lambda_\ell = \sum_{j=1}^{n-1} a_j \zeta_n^{j\ell}$, for $\ell \neq 0$. By definition of a_j,

$$\lambda_\ell = \sum_{j=1}^{n-1} \left(\frac{1}{\zeta_n^{-j} - 1} + \sum_{k=0}^{n-1} c_k \zeta_n^{-jk} \right) \zeta_n^{j\ell} = \sum_{j=1}^{n-1} \frac{\zeta_n^{j\ell}}{\zeta_n^{-j} - 1} + c_\ell n - \sum_{k=0}^{n-1} c_k. \tag{48}$$

Using (47), we get

$$\lambda_\ell = \sum_{j=1}^{n-1} \frac{\zeta_n^{j\ell} - 1}{\zeta_n^{-j} - 1} + c_\ell n + \lambda_0 = (n-1) - \sum_{j=1}^{n-1} \frac{1 - \zeta_n^{j(\ell+1)}}{1 - \zeta_n^j} + c_\ell n + \lambda_0. \tag{49}$$

But, note that

$$\sum_{j=1}^{n-1} \frac{1 - \zeta_n^{j(\ell+1)}}{1 - \zeta_n^j} = \sum_{j=1}^{n-1} \sum_{s=0}^{\ell} \zeta_n^{sj} = n - 1 - \ell. \tag{50}$$

This shows that $\lambda_\ell = \ell + c_\ell n + \lambda_0$, for $\ell = 1, \dots, n-1$. By Theorem 5, this shows G has universal perfect state transfer.

Here, we confirm that the underlying graph of G is connected. Since $1 - \zeta_p^{-1}$ is not a unit of $\mathbb{Z}[\zeta_p]$, for any prime p, we have

$$a_q = \frac{1}{\zeta_n^{-q} - 1} + \sum_{k=0}^{n} c_k \zeta_n^{-qk} = \frac{1}{\zeta_p^{-1} - 1} + \sum_{k=0}^{n-1} c_k \zeta_p^{-k} \neq 0 \tag{51}$$

since c_k are all integers. Similarly, $a_p \neq 0$. Since $\gcd(p, q) = 1$, Fact 2 implies G is connected. □

Example 2. We show a circulant G of order $n = 6$ with universal perfect state transfer which is *not* dense. Here, we have $\zeta_6 = \frac{1}{2} + \mathtt{i}\frac{\sqrt{3}}{2}$, $\zeta_6^2 = -\frac{1}{2} + \mathtt{i}\frac{\sqrt{3}}{2}$, $\zeta_6^3 = -1$, $\zeta_6^4 = -\frac{1}{2} - \mathtt{i}\frac{\sqrt{3}}{2}$, $\zeta_6^5 = \frac{1}{2} - \mathtt{i}\frac{\sqrt{3}}{2}$. Note that

$$a_1 = \frac{1}{\zeta_6^{-1} - 1} + \sum_{k=0}^{5} c_k \zeta_6^{-k} = \frac{1}{\zeta_6^5 - 1} + (1 - \zeta_6) = 0. \tag{52}$$

So, in Theorem 6, we choose $c_0 = 1$, $c_1 = c_2 = c_3 = c_4 = 0$ and $c_5 = -1$. The other coefficients can be computed using $a_j = 1/(\zeta_6^{-1} - 1) + \sum_{k=0}^{5} c_k \zeta_6^{-jk}$. By a straightforward computation, $a_0 = \frac{5}{2}$, $a_2 = 1 - \frac{\mathtt{i}}{\sqrt{3}}$, $a_3 = \frac{3}{2}$, $a_4 = 1 + \frac{\mathtt{i}}{\sqrt{3}}$ and, of course, $a_5 = 0$.

Hence, the adjacency matrix of G is given by

$$\begin{bmatrix} \frac{5}{2} & 0 & 1 - \frac{\mathtt{i}}{\sqrt{3}} & \frac{3}{2} & 1 + \frac{\mathtt{i}}{\sqrt{3}} & 0 \\ 0 & \frac{5}{2} & 0 & 1 - \frac{\mathtt{i}}{\sqrt{3}} & \frac{3}{2} & 1 + \frac{\mathtt{i}}{\sqrt{3}} \\ 1 + \frac{\mathtt{i}}{\sqrt{3}} & 0 & \frac{5}{2} & 0 & 1 - \frac{\mathtt{i}}{\sqrt{3}} & \frac{3}{2} \\ \frac{3}{2} & 1 + \frac{\mathtt{i}}{\sqrt{3}} & 0 & \frac{5}{2} & 0 & 1 - \frac{\mathtt{i}}{\sqrt{3}} \\ 1 - \frac{\mathtt{i}}{\sqrt{3}} & \frac{3}{2} & 1 + \frac{\mathtt{i}}{\sqrt{3}} & 0 & \frac{5}{2} & 0 \\ 0 & 1 - \frac{\mathtt{i}}{\sqrt{3}} & \frac{3}{2} & 1 + \frac{\mathtt{i}}{\sqrt{3}} & 0 & \frac{5}{2} \end{bmatrix}. \tag{53}$$

The eigenvalues of G are given by $\lambda_k = \sum_{j=0}^{5} a_j \zeta_6^{jk}$. We confirm the eigenvalue form in (18) that $\lambda_\ell = \ell + 6c_\ell$, for $\ell = 0, 1, \dots, 5$. It can be verified that $\lambda_0 = 6 = 0 + 6c_0$, $\lambda_1 = 1 = 1 + 6c_1$, $\lambda_2 = 2 = 2 + 6c_2$, $\lambda_3 = 3 = 3 + 6c_3$, $\lambda_4 = 4 = 4 + 6c_4$, and $\lambda_5 = -1 = 5 + 6c_5$.

8. Property $\mathbb{T}$

In this concluding section, we consider universal perfect state transfer in complex unit gain graphs. First, we observe the following fact.

Fact 5. $\texttt{Circ}(0, -\texttt{i}, \texttt{i})$ is the only graph on 3 vertices with universal perfect state transfer, up to switching equivalence.

Proof. Cameron et al. [3] showed that $\texttt{Circ}(0, -\texttt{i}, \texttt{i})$ has universal perfect state transfer. Hence, it suffices to show that any graph on 3 vertices with universal perfect state transfer must be a circulant.

Let G be a graph with Hermitian adjacency matrix A. Suppose M is a type-II matrix of the form

$$M = \begin{bmatrix} 1 & 1 & 1 \\ 1 & e^{\texttt{i}\alpha} & e^{\texttt{i}\beta} \\ 1 & e^{\texttt{i}\beta} & e^{\texttt{i}\alpha} \end{bmatrix} \tag{54}$$

which diagonalizes A. By Corollary 1, we have that $1 + e^{\texttt{i}\alpha} + e^{\texttt{i}\beta} = 0$. This shows $\cos(\alpha) + \cos(\beta) = -1$ and $\sin(\alpha) + \sin(\beta) = 0$. This implies $\alpha = 2\pi/3$ and $\beta = 2\alpha$. Thus, $M/\sqrt{3}$ is the Fourier matrix which diagonalizes any circulant matrix of order 3. □

Godsil [9] proved that for any constant k, there is only a finite number of (unweighted) graphs with maximum degree k with perfect state transfer. This shows that perfect state transfer is a rare phenomenon (in the absence of weights). This motivates our next conjecture.

We say a graph has *property* $\mathbb{T}$ if all of the nonzero coefficients in its adjacency matrix are complex numbers with unit magnitude.

Conjecture 1. $\texttt{Circ}(0, -\texttt{i}, \texttt{i})$ *is the only circulant with property* $\mathbb{T}$ *which has universal perfect state transfer.*

Acknowledgements

Research supported by NSF grant DMS-1262737. Part of this work was started while C.T. was visiting Institut Henri Poincaré (Centre Émile Borel) and University of Waterloo. This author would like to thank IHP and Chris Godsil for hospitality and support.

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