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PERFECT STATE TRANSFER, GRAPH PRODUCTS AND EQUITABLE PARTITIONS

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We describe new constructions of graphs which exhibit perfect state transfer on continuous-time quantum walks. Our constructions are based on generalizations of the double cones and variants of the Cartesian graph products (which include the hypercube). We also describe a generalization of the path collapsing argument (which reduces questions about perfect state transfer to simpler weighted multigraphs) for graphs with equitable distance partitions.

Keywords: Perfect state transfer; quantum walk; graph product; equitable partition.

1. Introduction

Recently, perfect state transfer in continuous-time quantum walks on graphs has received considerable attention. This is due to its potential applications for the transmission of quantum information over quantum networks. It was originally

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introduced by Bose[1] in the context of quantum walks on linear spin chains or paths. Another reason for this strong interest is due to the universal property of quantum walks as a computational model as outlined by Childs.[2] From a graph-theoretic perspective, the main question is whether there is a spectral characterization of graphs which exhibit perfect state transfer. Strong progress along these lines were given on highly structured graphs by Bernasconi *et al.*[3] for hypercubic graphs and by Bašić and Petković[4] for integral circulants. Nevertheless, a general characterization remains elusive (see Godsil[5]).

Christandl *et al.*[6,7] showed that the n-fold Cartesian product of the one-link P_2 and two-link P_3 graphs admit perfect state transfer. This is simply because P_2 and P_3 have end-to-end perfect state transfer and the Cartesian product operator preserves perfect state transfer. They also drew a crucial connection between hypercubic networks and weighted paths using the so-called *path-collapsing* argument. This argument was also used by Childs *et al.*[8] in the context of an exponential algorithmic speedup for a black-box graph search problem via continuous-time quantum walks. Christandl *et al.*[7] proved that, although the n-vertex path P_n, for $n \geq 4$, has no end-to-end perfect state transfer, a suitably weighted version of P_n has perfect state transfer (via a path-collapsing reduction from the n-cube Q_n). A somewhat critical ingredient of this reduction is that each layer of Q_n is an empty graph. We generalize this argument to graphs which have equitable distance partitions (see Godsil and Royle[9]).

Bose *et al.*[10] observed an interesting phenomena on the complete graph K_n. Although K_n does not exhibit perfect state transfer, they show that by removing an edge between any two vertices, perfect state transfer is created between them. Note that the graph we obtain from removing an edge from K_n is the double cone $\overline{K}_2 + K_{n-2}$ (where $G + H$ denotes the join of graphs G and H). This phenomena was also observed by Tsomokos *et al.*[11] in relation to the cocktail party graph. This observation was generalized in Angeles-Canul *et al.*[12] where perfect state transfer was proved for double cones $\{\overline{K}_2, K_2\} + G$, where G is some regular graph (in place of complete graphs). The analyses on these double cones showed that perfect state transfer need not occur between antipodal vertices and that having integer eigenvalues is not a sufficient condition for perfect state transfer (which answered questions raised by Godsil[5]).

Our goal in this work is to combine and extend both the Cartesian product and the double cone constructions. The Cartesian product construction (which combines graphs with perfect state transfer) has the advantage of producing large diameter graphs with antipodal perfect state transfer. In fact, this construction provides the best upper bound for the order-diameter problem; for a given d, let $f(d)$ be the smallest size graph which has perfect state transfer between two vertices of distance d. Then, the best known bounds are $d \leq f(d) \leq \alpha^d$, where $\alpha = 2$, if d is odd, and $\alpha = \sqrt{3}$, if d is even; here, the upper bounds are achieved by $P_2^{\otimes n}$ and $P_3^{\otimes n}$. On the other hand, the double cone construction allows graphs whose quotients (modulo its equitable partition) contain cells which are not independent sets. This can potentially

allow for a broader class of graphs with perfect state transfer (see Bose *et al.*,[10] Tsomokos *et al.*,[11] and Angeles-Canul *et al.*[12,13]).

In this work, we describe new constructions of families of graphs with perfect state transfer. First, we extend several of the double cone constructions and relax their diameter restrictions. We show that the double cone $\overline{K}_2 + G$ of an arbitrary connected graph G has perfect state transfer if we use edge weights proportional to the Perron eigenvector of G. This extends results given in Ref. 12 where G is required to be a regular graph. Then, we prove that the glued double cone graph $K_1 + G_1 \circ G_2 + K_1$ has perfect state transfer whenever G_1, G_2 belongs to some class of regular graphs and if they are connected using some matrix C which commutes with the adjacency matrices of G_1 and G_2. In contrast, Angeles-Canul *et al.*[13] proved that $K_1 + G + G + K_1$ has no perfect state transfer, for any regular graph G, even if weights are allowed.

For cones with larger diameter, we consider the graph $K_1 + G_1 + H + G_2 + K_1$, where G_1, G_2 belong to the same class of regular graphs and H is another regular graph. This symmetry is a necessary condition for perfect state transfer as shown by Kay.[14] Nevertheless, in contrast to the previous positive results, we show there is no perfect state transfer whenever H is the empty graph. The 4-dimensional cube Q_4 (which has perfect state transfer) is an example of such a graph but without the join (or complete bipartite) connection.

Our other contribution involves constructions of perfect state transfer graphs using alternative graph products, namely the weak and lexicographic products. An interesting property of these products is that they can create perfect state transfer graphs by combining graphs with perfect state transfer and ones which lack the property. For example, we show that $Q_{2n} \times K_{2m}$ has perfect state transfer, for any integers n and m. Recall that the complete graph has no perfect state transfer (as observed by Bose *et al.*[10]). In comparison, the Cartesian product requires both of its graph arguments to have perfect state transfer (with the same perfect state transfer times). We also consider the lexicographic graph product (or graph composition) and its generalizations. Our generalized lexicographic product of G and H using a connection matrix (or graph) C is a graph $G_C[H]$ whose adjacency matrix is $A_G \otimes C + I \otimes A_H$. Note we recover the Cartesian product by letting $C = I$ and the standard lexicographic product by letting $C = J$. So, this generalization interpolates
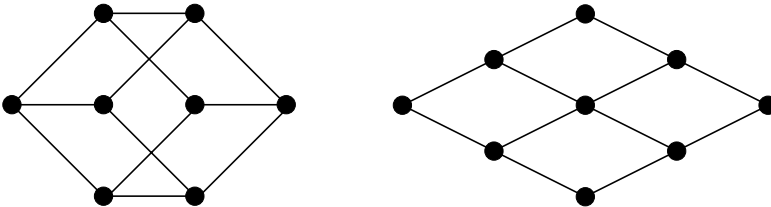

Fig. 1.   The Cartesian product construction for perfect state transfer (left to right): (a) $P_2 \oplus P_2 \oplus P_2$; (b) $P_3 \oplus P_3$ (see Christandl, Datta, Dorlas, Ekert, Kay, and Landahl, *Physical Review A* **71** (2005) 032312).

Graph family	PST	Construction	Source
$\{\overline{K}_2, K_2\} + \mathcal{G}$	yes	join	$10, 12$
$\{\overline{K}_2, K_2\} + \tilde{\mathcal{G}}$	yes*	join	this work
$P_{n \geq 4}$	no	path	7
$K_1 + \mathcal{G} \circ \mathcal{G} + K_1$	yes	circulant half-join	this work
$K_1 + \mathcal{G} + \mathcal{G} + K_1$	no*	half-join	13
$K_1 + \mathcal{G} + \overline{K}_n + \mathcal{G} + K_1$	no	join	this work
Q_n or $P^{\oplus n}$	yes	Cartesian product	7
$\{Q_{2n}, P_3^{\oplus n}\} \times$ ODD-CIRC	yes	weak product	this work
INT$[Q_{n \geq 2}]$	yes	lexicographic product	this work

Fig. 2.   *Summary of results on some graphs with perfect state transfer*: n is a positive integer; $\mathcal{G}$ denotes some family of regular graphs; $\tilde{\mathcal{G}}$ denotes an arbitrary connected graph; P_n is the path on n vertices; Q_n is the n-dimensional cube; K_n is the complete graph on n vertices; ODD-CIRC is the class of circulant graphs with odd eigenvalues; INT is the class of integral graphs. Asterisks indicate results on weighted graphs.

between these two known graph products. For example, we show that the lexicographic product $G[Q_n]$ has perfect state transfer for any integral graph G and $n \geq 2$.

The proofs we employ exploit elementary spectral properties of the underlying graphs. Some of our results are summarized in Fig. 2.

2. Preliminaries

Let $[n]$ denote the set $\{0, 1, \ldots, n-1\}$. For a tuple of binary numbers $(a, b) \in \{0, 1\}^2 \setminus \{(0, 0)\}$, let $\mathbb{Q}_{a,b}$ denote the set of rational numbers of the form p/q, with $gcd(p, q) = 1$, where $p \equiv a \pmod 2$ and $q \equiv b \pmod 2$. These denote rational numbers (in lowest terms) that are ratios of two odd integers or of an odd integer and an even integer, or vice versa. We denote the even and odd integers as $2\mathbb{Z}$ and $2\mathbb{Z} + 1$, respectively.

The graphs $G = (V, E)$ we study are finite, simple, undirected, connected, and mostly unweighted. The adjacency matrix A_G of a graph G is defined as $A_G[u, v] = 1$ if $(u, v) \in E$ and 0 otherwise; we also use $u \sim v$ to mean u is adjacent to v. The spectrum $\text{Spec}(G)$ of G is the set of eigenvalues of A_G. The graph G is called *integral* if all of its eigenvalues are integers. A graph $G = (V, E)$ is called k-regular if each vertex $u \in V$ has exactly k adjacent neighbors. For integers $n \geq 1$ and $0 \leq k < n$, let $\mathcal{G}_{n,k}$ be the set of all n-vertex k-regular graphs. The distance $d(a, b)$ between vertices a and b is the length of the shortest path connecting them.

Some standard graphs we consider include the complete graphs K_n, paths P_n, and circulants graphs. An n-vertex *circulant* graph G is a graph whose adjacency matrix is an $n \times n$ circulant matrix; that is, there is a sequence $(a_0, \ldots, a_{n-1})$ so that $A_G[j, k] = a_{k-j}$, where arithmetic on the indices is done modulo n. Alternatively, we may define a circulant graph G on $[n]$ through a subset $S \subseteq [n]$ where j is adjacent to k if and only if $k - j \in S$; we denote such a circulant as $Circ(n, S)$. Known examples of circulants include the complete graphs K_n and cycles C_n.

Let G and H be two graphs with adjacency matrices A_G and A_H, respectively. The complement of $G = (V, E)$, denoted $\overline{G} = (V, \overline{E})$, is a graph where $(u, v) \in \overline{E}$ if and only if $(u, v) \notin E$, for $u \neq v$. Some relevant binary graph operations are defined in the following:

- The *Cartesian product* $G \oplus H$ is a graph defined on $V(G) \times V(H)$ where (g_1, h_1) is adjacent to (g_2, h_2) if either $g_1 = g_2$ and $(h_1, h_2) \in E_H$, or $(g_1, g_2) \in E_G$ and $h_1 = h_2$. The adjacency matrix of $G \oplus H$ is $A_G \otimes I + I \otimes A_H$.
- The *weak product* $G \times H$ is a graph defined on $V(G) \times V(H)$ where (g_1, h_1) is adjacent to (g_2, h_2) if $(g_1, g_2) \in E_G$ and $(h_1, h_2) \in E_H$. The adjacency matrix of $G \times H$ is $A_G \otimes A_H$.
- The *lexicographic product* $G[H]$ is a graph defined on $V(G) \times V(H)$ where (g_1, h_1) is adjacent to (g_2, h_2) if either $(g_1, g_2) \in E_G$ or $g_1 = g_2$ and $(h_1, h_2) \in E_H$. The adjacency matrix of $G[H]$ is $A_G \otimes J + I \otimes A_H$.
- The *join* $G + H$ is a graph defined on $V(G) \cup V(H)$ obtained by taking two disjoint copies of G and H and by connecting all vertices of G to all vertices of H. The adjacency matrix of $G + H$ is $\begin{bmatrix} A_G & J \\ J & A_H \end{bmatrix}$.

We assume appropriate dimensions on the identity I and all-one J matrices used above. The n-dimensional hypercube Q_n may be defined recursively as $Q_1 = K_2$ and $Q_n = K_2 \oplus Q_{n-1}$, for $n \geq 2$. The *cone* of a graph G is defined as $K_1 + G$. The *double cone* of G is $\overline{K}_2 + G$, whereas the *connected* double cone is $K_2 + G$.

A partition π of a graph $G = (V, E)$ given by $V = \uplus_{j=1}^m V_j$ is called *equitable* if the number of neighbors in V_k of a vertex u in V_j is a constant $d_{j,k}$, independent of u (see the monographs by Godsil and Royle[9] and by Godsil[15]). The *quotient* graph of G over π, denoted by G/π, is the directed graph with the m cells of π as its vertices and $d_{j,k}$ edges from the jth to the kth cells of π. The adjacency matrix of G/π is given by $A_{G/\pi}[j, k] = d_{j,k}$.

A graph G has an *equitable distance partition* π with respect to a vertex a if $\pi = \uplus_{j=0}^m V_j$ is such that G/π is a *path* and $V_j = \{x \in V : d(x, a) = j\}$ where $V_0 = \{a\}$; typically, we also require that there is a vertex b, antipodal to a, so that $V_m = \{b\}$. We also call a graph a *cylindrical cone* (see Fig. 3) if it has an equitable distance partition and is denoted $K_1 \circ G_1 \circ, \ldots, \circ G_m \circ K_1$, where G_j are regular graphs and $\circ$ denote (semi-)regular bipartite connections (induced by the equitable partition π).
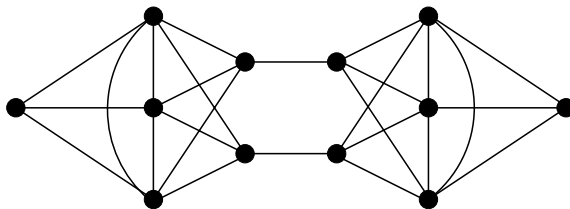

Fig. 3.   A cylindrical cone with an equitable distance partition: $K_1 + K_3 \circ \overline{K}_2 \circ \overline{K}_2 \circ K_3 + K_1$.

Further background on algebraic graph theory may be found in the comprehensive texts by Biggs,[16] Godsil and Royle,[9] and Godsil.[15]

Next, we describe the continuous-time quantum walk as defined originally by Farhi and Gutmann.[17] For a graph $G = (V, E)$, let $|\psi(0)\rangle \in \mathbb{C}^{|V|}$ be an initial amplitude vector of unit length. Using Schrödinger's equation, the amplitude vector of the quantum walk at time t is

$$|\psi(t)\rangle = e^{-itA_G}|\psi(0)\rangle. \tag{1}$$

Note that since A_G is Hermitian (in our case, symmetric), e^{-itA_G} is unitary (hence, an isometry). More detailed discussion of quantum walks on graphs can be found in the excellent surveys by Kempe[18] and Kendon.[19] The *instantaneous* probability of vertex a at time t is $p_a(t) = |\langle a|\psi(t)\rangle|^2$. We say G has *perfect state transfer* from vertex a to vertex b at time t if a continuous-time quantum walk on G from a to b has unit fidelity or

$$|\langle b|e^{-itA_G}|a\rangle| = 1, \tag{2}$$

where $|a\rangle$, $|b\rangle$ denote the unit vectors corresponding to the vertices a and b, respectively. The graph G has perfect state transfer if there exist vertices a and b in G and time t so that (2) is true.

3. Graph Products

In this section, we describe constructions of perfect state transfer graphs using the weak and lexicographic products. These complement the well-known Cartesian product constructions (see Christandl *et al.*[6,7]).

3.1. *Weak product*

An interesting property of the weak product graph operator is that it can create graphs with perfect state transfer by combining ones with perfect state transfer and ones which lack the property. In contrast, the Cartesian graph product can only create perfect state transfer graphs from ones which have the property. We start with the following simple observation.

Fact 1. Let G be an n-vertex graph and H be an m-vertex graph whose eigenvalues and eigenvectors are given by $A_G|u_k\rangle = \lambda_k|u_k\rangle$, for $k \in [n]$, and $A_H|v_\ell\rangle = \mu_\ell|v_\ell\rangle$, for $\ell \in [m]$, respectively. Let $g_1, g_2 \in V_G$ and $h_1, h_2 \in V_H$. Then, the fidelity of a quantum walk on their weak product $G \times H$ between (g_1, h_1) and (g_2, h_2) is given by

$$\langle g_2, h_2|e^{-itA_{G \times H}}|g_1, h_1\rangle$$

$$= \langle g_2| \left[\sum_k \left\{ \sum_\ell \langle h_2|v_\ell\rangle\langle v_\ell|h_1\rangle e^{-it\lambda_k\mu_\ell} \right\} |u_k\rangle\langle u_k| \right] |g_1\rangle. \tag{3}$$
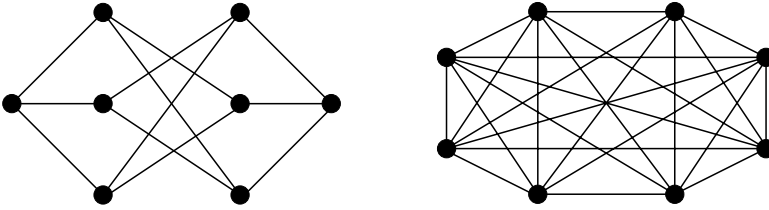
Fig. 4. Graph products with perfect state transfer (left to right): (a) the weak product $K_2 \times K_{4m}$, for $m \geq 1$ (shown here with $m = 1$); (b) the lexicographic product (or composition) $K_m[Q_n]$ (shown here with $m = n = 2$).

Proof. Recall that the adjacency matrix of $A_{G \times H}$ is $A_G \otimes A_H$. Thus, the eigenvalues and eigenvectors of the weak product $G \times H$ are

$$A_{G \times H}(|u_k\rangle \otimes |v_\ell\rangle) = \lambda_k \mu_\ell (|u_k\rangle \otimes |v_\ell\rangle), \quad \text{where } k \in [n] \text{ and } \ell \in [m]. \qquad (4)$$

So, the quantum walk on $G \times H$ from (g_1, h_1) to (g_2, h_2) is given by

$$\langle g_2, h_2 | e^{-itA_{G \times H}} | g_1, h_1 \rangle = \sum_{k, \ell} \langle g_2 | u_k \rangle \langle u_k | g_1 \rangle \langle h_2 | v_\ell \rangle \langle v_\ell | h_1 \rangle e^{-it\lambda_k \mu_\ell}. \qquad (5)$$

After rearranging summations, we obtain the claim. $\qquad \square$

Proposition 1. *Let G be a graph with perfect state transfer at time t_G so that*

$$t_G \text{Spec}(G) \subseteq \mathbb{Z}\pi. \qquad (6)$$

Then, $G \times H$ has perfect state transfer if H is a circulant graph with odd eigenvalues.

Proof. Suppose G is an n-vertex graph whose eigenvalues and eigenvectors are given by $A_G |u_k\rangle = \lambda_k |u_k\rangle$, for $k \in [n]$. Assume that G has perfect state transfer at time t_G from vertex g_1 to g_2. Also, suppose H be an m-vertex graph whose eigenvalues and eigenvectors are given by $A_H |v_\ell\rangle = \mu_\ell |v_\ell\rangle$, for $\ell \in [m]$. In Eq. (3), if H is circulant on m vertices, we have $\langle 0 | v_\ell \rangle \langle v_\ell | 0 \rangle = 1/m$. Moreover, if each eigenvalue of H is odd, say $\mu_\ell = 2m_\ell + 1$, with $m_\ell \in \mathbb{Z}$, then

$$\langle g_2, 0 | \exp(-it_G A_{G \times H}) | g_1, 0 \rangle = \frac{1}{m} \sum_{k, \ell} \langle g_2 | u_k \rangle \langle u_k | g_1 \rangle e^{-it_G \lambda_k \mu_\ell} \qquad (7)$$

$$= \frac{1}{m} \sum_k \langle g_2 | u_k \rangle \langle u_k | g_1 \rangle \sum_\ell e^{-it_G \lambda_k (2m_\ell + 1)} \qquad (8)$$

$$= \sum_k \langle g_2 | u_k \rangle \langle u_k | g_1 \rangle e^{-it_G \lambda_k}, \quad \text{since } t_G \lambda_k \in \mathbb{Z}\pi. \qquad (9)$$

The last expression equals to $\langle g_2 | e^{-it_G A_G} | g_1 \rangle$, by the spectral theorem. This proves the claim. $\qquad \square$

Remark. Note Q_{2n} has eigenvalues $\lambda_k = 2n - 2k$, for $k = 0, \ldots, 2n$, and perfect state transfer time $t = \pi/2$. Also, $P_3^{\otimes n}$ has eigenvalues from $\lambda_k \in \mathbb{Z}\sqrt{2}$ and perfect state

transfer time $t = \pi/\sqrt{2}$. In both cases, we have $t\lambda_k \in \mathbb{Z}\pi$, for all k. Thus, by Proposition 1, we find that $\{Q_{2n}, P_3^{\otimes n}\} \times H$ has perfect state transfer for any circulant H with odd eigenvalues. For example, we may let $H = K_m$ be the complete graph of order m, for an even integer m.

3.2. *Lexicographic products*

The generalized lexicographic product $G_C[H]$ between a graph G and two graphs H and C, with $V_H = V_C$, is a graph on $V_G \times V_H$ where (g_1, h_1) is adjacent to (g_2, h_2) if and only if either $(g_1, g_2) \in E_G$ and $(h_1, h_2) \in E_C$, or, $g_1 = g_2$ and $(h_1, h_2) \in E_H$. In terms of adjacency matrices, we have

$$A_{G_C[H]} = A_G \otimes A_C + I \otimes A_H. \tag{10}$$

We describe constructions of perfect state transfer graphs using generalized lexicographic products. Again, we start with the following simple observation.

Fact 2. Let G be an n-vertex graph whose eigenvalues and eigenvectors are given by $A_G|u_k\rangle = \lambda_k|u_k\rangle$, for $k \in [n]$. Let H and C be m-vertex graphs whose adjacency matrices commute, that is $[A_H, A_C] = 0$, and whose eigenvalues and eigenvectors are given by $A_H|v_\ell\rangle = \mu_\ell|v_\ell\rangle$, and $A_C|v_\ell\rangle = \gamma_\ell|v_\ell\rangle$, for $\ell \in [m]$, respectively. Suppose g_1, $g_2 \in V_G$ and $h_1, h_2 \in V_H$. Then, the fidelity of a quantum walk on the generalized lexicographic product $G_C[H]$ between (g_1, h_1) and (g_2, h_2) is given by

$$\langle g_2, h_2 | \exp(-itA_{G_C[H]}) | g_1, h_1 \rangle$$
$$= \sum_k \langle g_2|u_k\rangle\langle u_k|g_1\rangle \sum_\ell \langle h_2|v_\ell\rangle\langle v_\ell|h_1\rangle e^{-it(\lambda_k\gamma_\ell + \mu_\ell)}. \tag{11}$$

Proof. The eigenvalues and eigenvectors of $G_C[H]$ are given by

$$A_{G_C[H]}(|u_k\rangle \otimes |v_\ell\rangle) = (\lambda_k\gamma_\ell + \mu_\ell)(|u_k\rangle \otimes |v_\ell\rangle), \quad k \in [n] \quad \text{and} \quad \ell \in [m]. \tag{12}$$

So, the quantum walk on $G_C[H]$ from (g_1, h_1) to (g_2, h_2) is given by

$$\langle g_2, h_2 | e^{-itA_{G_C[H]}} | g_1, h_1 \rangle = \sum_{k,\ell} \langle g_2|u_k\rangle\langle u_k|g_1\rangle\langle h_2|v_\ell\rangle\langle v_\ell|h_1\rangle e^{-it(\lambda_k\gamma_\ell + \mu_\ell)}, \tag{13}$$

which proves the claim.   □

In the following, we show a closure property of perfect state transfer graphs using a generalized lexicographic product with the complete graph as a connection matrix. This is similar to the weak product construction from Proposition 1.

Proposition 2. *Let G and H be perfect state transfer graphs with a common time t. Assume that H is a m-vertex graph which commutes with K_m. Suppose that*

$$t|V_H|\mathrm{Spec}(G) \subseteq 2\mathbb{Z}\pi. \tag{14}$$

Then, the lexicographic product $G_{K_m}[H]$ has perfect state transfer at time t.

Proof. Suppose G has perfect state transfer from g_1 to g_2 at time t, where $g_1, g_2 \in V_G$. Let the eigenvalues and eigenvectors of G be given by $A_G|u_k\rangle = \lambda_k|u_k\rangle$, for $k \in [n]$. Also, suppose H is a circulant with perfect state transfer from h_1 to h_2 at time t, where $h_1, h_2 \in V_H$. Let the eigenvalues and eigenvectors of H be given by $A_H|v_\ell\rangle = \mu_\ell|\mu_\ell\rangle$, for $\ell \in [m]$. Thus, Eq. (11) becomes

$$\langle g_2, h_2|e^{-itA_{G_{K_m}[H]}}|g_1, h_1\rangle \tag{15}$$

$$= \sum_k \langle g_2|u_k\rangle\langle u_k|g_1\rangle \tag{16}$$

$$\times \left[e^{-it(\lambda_k(m-1)+\mu_0)}\langle h_2|v_0\rangle\langle v_0|h_1\rangle + \sum_{\ell \neq 0} e^{-it(-\lambda_k+\mu_\ell)}\langle h_2|v_\ell\rangle\langle v_\ell|h_1\rangle \right] \tag{17}$$

$$= \langle g_2|e^{itA_G}|g_1\rangle\langle h_2|e^{-itA_H}|h_1\rangle, \tag{18}$$

since $e^{-it(m-1)\lambda_k} = e^{it\lambda_k}$, for all k. This shows that $G_{K_m}[H]$ has perfect state transfer from (g_1, h_1) to (g_2, h_2) at time t. $\qquad\square$

The *standard* lexicographic product $G[H]$ is obtained when we let $C = J$ in Eq. (10). In this case, Eq. (11) decouples nicely and we have a similar result to Proposition 2 but without requiring G to have perfect state transfer.

Lemma 1. *Let G be an arbitrary graph and let H be a regular graph with perfect state transfer at time t_H from h_1 to h_2, for $h_1, h_2 \in V_H$. Then, $G[H]$ has perfect state transfer from (g, h_1) to (g, h_2), for any $g \in V_G$, if*

$$t_H|V_H|\mathrm{Spec}(G) \subseteq 2\mathbb{Z}\pi. \tag{19}$$

Proof. If H is an m-vertex regular graph, then $[A_H, J_m] = 0$. The all-one matrix J_m has eigenvalues m (with multiplicity one) and 0 (with multiplicity $m-1$). Thus, Eq. (11) becomes

$$\langle g, h_2|e^{-it_H A_{G[H]}}|g, h_1\rangle \tag{20}$$

$$= \sum_k \langle g|u_k\rangle\langle u_k|g\rangle \left[e^{-it_H(\lambda_k m+\mu_0)}\langle h_2|v_0\rangle\langle v_0|h_1\rangle + \sum_{\ell \neq 0} e^{-it_H\mu_\ell}\langle h_2|v_\ell\rangle\langle v_\ell|h_1\rangle \right] \tag{21}$$

$$= \langle h_2|e^{-it_H A_H}|h_1\rangle, \tag{22}$$

since $e^{-it_H m\lambda_k(G)} = 1$, for all k, and $\sum_k |u_k\rangle\langle u_k| = I$. This proves the claim. $\qquad\square$

Remark. We will adopt the convention of scaling quantum walk time with respect to the *size* of the underlying graphs. Moore and Russell[20] proved that a continuous-time quantum walk on the n-cube Q_n has a uniform mixing time of $(2\mathbb{Z}+1)(\pi/4)n$ (which shows the time scaling with respect to the dimension of the n-cube). They used $H = (1/n)A_{Q_n}$ as their Hamiltonian — which is the probability transition matrix of the simple random walk on Q_n.

Corollary 1. *Suppose H is a k_H-regular graph with perfect state transfer at time $t_H = (\pi/2)k_H$ and G is an integral graph (all of its eigenvalues are integers). Then, $G[H]$ has perfect state transfer provided $k_H|V_H|\mathrm{Spec}(G) \subseteq 4\mathbb{Z}$.*

Proof. Apply Lemma 1 by noting that $e^{-it_H |V_H| \lambda_k(G)} = 1$, since $t_H = (\pi/2) k_H$ and $\lambda_k(G) k_H |V_H|$ is divisible by 4, for all k. $\qquad\square$

The n-cube Q_n is a n-regular graph on 2^n vertices which has perfect state transfer at time $n(\pi/2)$ (with time scaling) (see Ref. 3). Thus, for any integral graph G, the composition graph $G[Q_n]$ has perfect state transfer if $n \geq 2$.

4. Cones

In this section, we explore some constructions of perfect state transfer graphs which generalize the double cones studied by Bose *et al.*,[10] Tsomokos *et al.*,[11] and Angeles-Canul *et al.*[12,13] The goal behind these constructions is to understand the types of intermediate graphs which allow perfect state transfer between the two antipodal vertices. For the double cones $\{K_2, \overline{K}_2\} + \mathcal{G}_{n,k}$, the intermediate graphs are n-vertex k-regular graphs and sufficient conditions for perfect state transfer on n and k were derived by Angeles-Canul *et al.*[12]

Here, we consider more complex cones by allowing irregular graphs (on double cones), by increasing the number of intermediate layers, and by varying the connectivity structure (using semi-regular bipartite connections). We show new perfect state transfer graphs for irregular double cones and for double half-cones with circulant connections, and also prove negative results for longer diameter cones on join connections.

4.1. *Irregular double cones*

We recall the Perron-Frobenius theory of nonnegative matrices. A matrix is called *nonnegative* if it has no negative entries. The spectral radius of a matrix A, denoted $\rho(A)$, is the maximum eigenvalue of A (in absolute value). The Perron-Frobenius theorem for nonnegative matrices states that if A is a real nonnegative $n \times n$ matrix whose underlying directed graph G is strongly connected, then $\rho = \rho(A)$ is a simple eigenvalue of A; moreover, the unique eigenvector corresponding to ρ has no zero entries and all entries have the same sign.

In what follows, we denote K_2^b as the two-vertex graph which equals K_2 if $b = 1$, and equals $\overline{K}_2$ if $b = 0$.

Theorem 3. *Let G be any connected graph whose maximum (simple) eigenvalue is λ_0 with a corresponding positive (normalized) eigenvector $|x_0\rangle$. Consider the double cone $\mathcal{G} = K_2^b + G$, for $b \in \{0, 1\}$, where the edges adjacent to the vertices of K_2^b, say A and B, are weighted proportional to $\alpha |x_0\rangle$. Then, the fidelity between A and B is given by*

$$\langle B | e^{-it A_\mathcal{G}} | A \rangle = \frac{1}{2} \left\{ e^{-it\tilde{\lambda}_0^+} \left[\cos(t\Delta) + i \frac{\tilde{\lambda}_0^-}{\Delta} \sin(t\Delta) \right] - 1 \right\}, \qquad (23)$$

where $\tilde{\lambda}_0^{\pm} = (\lambda_0 \pm b)/2$ and $\Delta = \sqrt{(\tilde{\lambda}_0^-)^2 + 2\alpha^2}$. Thus, perfect state transfer is achieved if $\tilde{\lambda}_0^+ / \Delta \in \mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,0}$.

Proof. Let A_G be the adjacency matrix of G. The adjacency matrix of $\mathcal{G}$ is

$$A_{\mathcal{G}} = \begin{bmatrix} 0 & b & \alpha\langle x_0| \\ b & 0 & \alpha\langle x_0| \\ \alpha|x_0\rangle & \alpha|x_0\rangle & A_G \end{bmatrix}. \tag{24}$$

For $1 \le k \le n-1$, let λ_k and $|x_k\rangle$ be the other eigenvalues and eigenvectors of A_G. Next, we define the following quantities:

$$\tilde{\lambda}_0^\pm = \frac{\lambda_0 \pm b}{2}, \quad \Delta = \sqrt{(\tilde{\lambda}_0^-)^2 + 2\alpha^2}, \quad \lambda_\pm = \tilde{\lambda}_0^+ \pm \Delta, \quad \kappa_\pm = \tilde{\lambda}_0^- \pm \Delta. \tag{25}$$

The eigenvalues of $A_{\mathcal{G}}$ are given by $\lambda_0 = 0$, $\lambda_\pm$, and λ_k, $1 \le k \le n-1$, with corresponding eigenvectors

$$|z_0\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} +1 \\ -1 \\ |0_n\rangle \end{bmatrix}, \quad |z_\pm\rangle = \frac{1}{L_\pm} \begin{bmatrix} \alpha/\kappa_\pm \\ \alpha/\kappa_\pm \\ |x_0\rangle \end{bmatrix}, \quad |z_k\rangle = \begin{bmatrix} 0 \\ 0 \\ |x_k\rangle \end{bmatrix} \tag{26}$$

where $L_\pm^2 = 2\alpha^2/\kappa_\pm^2 + 1$. Note $(\kappa_\pm L_\pm)^2 = 2\alpha^2 + \kappa_\pm^2 = 2\Delta(\Delta \pm \tilde{\lambda}_0^-)$. The fidelity between A and B, namely $\langle B|e^{-itA_{\mathcal{G}}}|A\rangle$, is given by

$$\sum_\pm \frac{\alpha^2 e^{-it\lambda_\pm}}{(\kappa_\pm L_\pm)^2} - \frac{1}{2} = \frac{1}{2}\left\{ \frac{(\Delta - \tilde{\lambda}_0^-)e^{-it(\tilde{\lambda}_0^+ + \Delta)} + (\Delta + \tilde{\lambda}_0^-)e^{-it(\tilde{\lambda}_0^+ - \Delta)}}{2\Delta} - 1 \right\} \tag{27}$$

$$= \frac{1}{2}\left\{ e^{-it\tilde{\lambda}_0^+}\left[\cos(t\Delta) + i\frac{\tilde{\lambda}_0^-}{\Delta}\sin(t\Delta) \right] - 1 \right\}. \tag{28}$$

For perfect state transfer to occur, it is sufficient to have $\tilde{\lambda}_0^+/\Delta \in \mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,0}$. $\qquad\square$

Corollary 2. *Let G be any connected graph whose maximum (simple) eigenvalue is λ_0 with corresponding positive eigenvector $|x_0\rangle$. Consider the double cone $\mathcal{G} = \overline{K}_2 + G$ where the edges adjacent to the two vertices of $\overline{K}_2$, say A and B, are weighted according to $\sqrt{n}|x_0\rangle$. Then, perfect state transfer exists from A to B if*

$$\frac{\lambda_0}{\sqrt{\lambda_0^2 + 8n}} \in \mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,0}. \tag{29}$$

Proof. In Theorem 3 with $b = 0$, let $\alpha = \sqrt{n}$ and note $\tilde{\lambda}_0^\pm = \lambda_0/2$. Thus, $\tilde{\lambda}_0^+/\Delta = \lambda_0/\sqrt{\lambda_0^2 + 8n}$, which proves the claim. $\qquad\square$

Remark. Given n, we may choose $\lambda_0 = \sqrt{8n/3}$ so the sufficient condition $\lambda_0/\sqrt{\lambda_0^2 + 8n} = 1/2$ is satisfied for perfect state transfer. Moreover, we can find a uniform edge weighting for G so that $\sqrt{8n/3}$ is a dominant eigenvalue. Thus, in the presence of weights, any double cone $\overline{K}_2 + G$ has perfect state transfer.
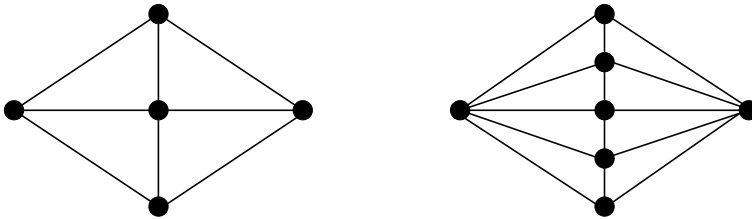
Fig. 5. Irregular weighted double cones have perfect state transfer (left to right): (a) $\overline{K}_2 + P_3$; (b) $\overline{K}_2 + P_5$.

4.2. *Glued double cones*

Analogous to the construction of glued-(binary)trees in Childs *et al.*,[8] we consider gluing two double cones using a semi-regular bipartite connection to obtain a perfect state transfer graph. In contrast, gluing two double cones using the join (full bipartite) connection yields no perfect state transfer (even with weights) as proved by Angeles-Canul *et al.*[13]

Theorem 4. *Let $G \in \mathcal{G}_{n,k}$ and let C be a symmetric Boolean matrix which commutes with the adjacency matrix of G. Suppose that $C|1_n\rangle = \gamma|1_n\rangle$. Let $k_\pm = 1/2(k \pm \gamma)$ and $\Delta_\pm = \sqrt{k_\pm + n}$. Then, the graph $\mathcal{G} = K_1 + G \circ G + K_1$, formed by taking two copies of $K_1 + G$ and connecting the copies of G using C, has perfect state transfer if $\Delta_+/\Delta_- \in \mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,0}$ and at least one of γ/Δ_+ or γ/Δ_- is in $\mathbb{Q}_{0,1}$.*

Proof. Suppose the eigenvalues and eigenvectors of G are λ_k and $|v_k\rangle$, respectively, where $k = \lambda_0 > \lambda_1 \geq \cdots \geq \lambda_{n-1}$. The adjacency matrix of $\mathcal{G}$ is given by

$$A_{\mathcal{G}} = \begin{bmatrix} 0 & 0 & \langle 1_n| & \langle 0_n| \\ 0 & 0 & \langle 0_n| & \langle 1_n| \\ |1_n\rangle & |0_n\rangle & A_G & C \\ |0_n\rangle & |1_n\rangle & C & A_G \end{bmatrix}. \tag{30}$$

Let $k_\pm = 1/2(k \pm \gamma)$ and $\Delta_\pm^2 = k_\pm^2 + n$. Let $\alpha_\pm = k_+ \pm \Delta_+$ and $\beta_\pm = k_- \pm \Delta_-$. The eigenvalues of $A_{\mathcal{G}}$ are given by $\alpha_\pm$, $\beta_\pm$, and $\pm\lambda_k$, for $k \neq 0$, with corresponding eigenvectors:

$$|\alpha_\pm\rangle = \frac{1}{L_\pm} \begin{bmatrix} 1 \\ 1 \\ \frac{1}{n}\alpha_\pm|1_n\rangle \\ \frac{1}{n}\alpha_\pm|1_n\rangle \end{bmatrix}, \quad |\beta_\pm\rangle = \frac{1}{M_\pm} \begin{bmatrix} +1 \\ -1 \\ +\frac{1}{n}\beta_\pm|1_n\rangle \\ -\frac{1}{n}\beta_\pm|1_n\rangle \end{bmatrix}, \quad |\lambda_k\rangle = \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ |v_k\rangle \\ \pm|v_k\rangle \end{bmatrix}, \tag{31}$$

where $L_\pm^2 = \frac{2}{n}(n + \alpha_\pm^2)$ and $M_\pm^2 = \frac{2}{n}(n + \beta_\pm^2)$ are the normalization constants. The quantum walks between involving the cone vertices, say A and B, are given by

$$\langle B|e^{-itA_{\mathcal{G}}}|A\rangle = \sum_\pm \frac{e^{-it\alpha_\pm}}{L_\pm^2} - \sum_\pm \frac{e^{-it\beta_\pm}}{M_\pm^2}, \tag{32}$$

$$\langle A|e^{-itA_{\mathcal{G}}}|A\rangle = \sum_\pm \frac{e^{-it\alpha_\pm}}{L_\pm^2} + \sum_\pm \frac{e^{-it\beta_\pm}}{M_\pm^2}. \tag{33}$$

At time $t = 0$, the second equation yields $1 = \sum_\pm L_\pm^{-2} + \sum_\pm M_\pm^{-2}$. To achieve perfect state transfer, it suffices to require

$$e^{-it\alpha_\pm} = +1, \quad e^{-it\beta_\pm} = -1, \quad e^{-it\gamma/2} = \pm 1. \tag{34}$$

We may restate these conditions as $\Delta_+/\Delta_- = \mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,0}$ and $\{\gamma/\Delta_+, \gamma/\Delta_-\} \cap \mathbb{Q}_{0,1} \neq \emptyset$. $\qquad\square$

Remark. In Theorem 4, the result also holds if we replace G with two distinct graphs G_1 and G_2 from the same family $\mathcal{G}_{n,k}$.

In the following corollary, we describe an explicit family of glued double cones which exhibit perfect state transfer. The construction uses a pair of circulant families of graphs (see Fig. 6).

Corollary 3. *For $a \geq 2$, let $n = 15 \times 2^{2(a-2)}$, $k = 3 \times 2^{a-1}$, and $\gamma = 4 \times 2^{a-1}$. Consider two circulant graphs $G = Circ(n, [k/2])$ and $C = Circ(n, [\gamma/2])$. Then, the graph $\mathcal{G} = K_1 + G \circ G + K_1$ has perfect state transfer, where the connection $\circ$ is specified by C.*

Proof. Note we have $k_\pm = 1/2(k \pm \gamma) = 2^{a-2}(3 \pm 4)$ and $\Delta_\pm = 2^{a-2}((3 \pm 4)^2 + 15) \in 2^{a-2}\{8, 4\}$. Thus, $\Delta_+/\Delta_- = 2 \in \mathbb{Q}_{0,1}$ and $\gamma/\Delta_- = 2 \in \mathbb{Q}_{0,1}$, which satisfy the sufficiency conditions for perfect state transfer in Theorem 4. $\qquad\square$

4.3. *Cylindrical cones*

In this section, we consider graphs of the form $K_1 + G_1 + H + G_2 + K_1$, where G_1, $G_2 \in \mathcal{G}_{n,k}$ and $H \in \mathcal{G}_{m,\ell}$. We show a negative result for perfect state transfer whenever
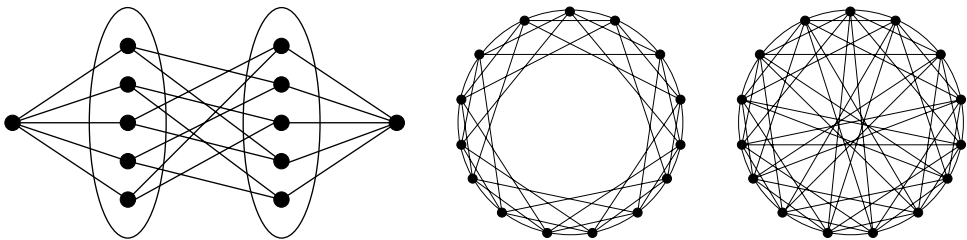

Fig. 6. Glued cones (left to right): (a) $K_1 + G \circ G + K_1$ has perfect state transfer, with (b) $G = Circ(15, \{1, 2, 4\})$; (c) $C = Circ(15, \{1, 2, 4, 7\})$. The connection $\circ$ is defined by C.

H is the empty graph. This generalizes known negative results on P_4 and $K_1 + G + G + K_1$ (see Christandl *et al.*[7] and Angeles-Canul *et al.*[13]).

Theorem 5. *For any integers n, k, m where $n \geq 1, 0 \leq k < n$, and $m \geq 1$, the graph $K_1 + G_1 + \overline{K}_m + G_2 + K_1$ has no perfect state transfer, whenever $G_1, G_2 \in \mathcal{G}_{n,k}$.*

Proof. Let $\mathcal{G}$ be the graph $K_1 + G_1 + H + G_2 + K_1$, where $G_1, G_2 \in \mathcal{G}_{n,k}$ and $H \in \mathcal{G}_{m,\ell}$. Let A_{G_1} be the adjacency matrix of G_1 with eigenvalues α_r and eigenvectors $|u_r\rangle$; similarly, let A_{G_2} be the adjacency matrix of G_2 with eigenvalues β_r and eigenvectors $|v_r\rangle$, for $r \in [n]$. Note $k = \alpha_0 = \beta_0$ are the simple maximum eigenvalues of both G_1 and G_2. Let A_H be the adjacency matrix of H with eigenvalues ρ_s and eigenvectors $|w_s\rangle$, where $\ell = \rho_0$ is the simple maximum eigenvalue of H. Thus, the adjacency matrix of $\mathcal{G}$ is given by

$$A_{\mathcal{G}} = \begin{bmatrix} 0 & 0 & \langle 1_n | & \langle 0_n | & \langle 0_n | \\ 0 & 0 & \langle 0_n | & \langle 0_n | & \langle 1_n | \\ |1_n\rangle & |0_n\rangle & A_{G_1} & J_{n,m} & O_{n,n} \\ |0_m\rangle & |0_m\rangle & J_{m,n} & A_H & J_{m,n} \\ |0_n\rangle & |1_n\rangle & O_{n,n} & J_{n,m} & A_{G_2} \end{bmatrix}. \tag{35}$$

In our case, we have $A_H = O_{m,m}$ is the zero $m \times m$ matrix and $\ell = 0$.

Let $\lambda_\pm$ be the roots of quadratic polynomial $\lambda^2 - k\lambda - n = 0$; thus $\lambda_\pm = \tilde{k} \pm \Delta$, where $\tilde{k} = k/2$ and $\Delta^2 = \tilde{k}^2 + n$. Consider roots of the cubic polynomial $(\mu - \ell)(\mu^2 - k\mu - (2m+1)n) - 2\ell m n = 0$. For $\ell = 0$, zero is a root of this cubic along with the two roots of the quadratic equation $\mu^2 - k\mu - (2m+1)n = 0$. Let $\mu_\pm = \tilde{k} \pm \Gamma$, where $\Gamma^2 = \tilde{k}^2 + (2m+1)n$. The eigenvalues of $A_{\mathcal{G}}$ are given by $\lambda_\pm$, $\mu_\pm$, 0, and $\lambda_r^{(1)}$, $\lambda_r^{(3)}$, for $r \neq 0$, and $\lambda_s^{(2)}$, for $s \neq 0$, with corresponding eigenvectors:

$$|\lambda_\pm\rangle = \frac{1}{L_\pm} \begin{bmatrix} +1 \\ -1 \\ +\frac{1}{n}\lambda_\pm|1_n\rangle \\ |0_n\rangle \\ -\frac{1}{n}\lambda_\pm|1_n\rangle \end{bmatrix}, \quad |\mu_\pm\rangle = \frac{1}{M_\pm} \begin{bmatrix} 1 \\ 1 \\ \frac{1}{n}\mu_\pm|1_n\rangle \\ 2|1_n\rangle \\ \frac{1}{n}\mu_\pm|1_n\rangle \end{bmatrix}, \quad |v_0\rangle = \frac{1}{N} \begin{bmatrix} 1 \\ 1 \\ |0_n\rangle \\ -1/m|1_n\rangle \\ |0_n\rangle \end{bmatrix}, \tag{36}$$

and

$$|\lambda_r^{(1)}\rangle = \begin{bmatrix} 0 \\ 0 \\ |u_r\rangle \\ |0_m\rangle \\ |0_n\rangle \end{bmatrix}, \quad |\lambda_s^{(2)}\rangle = \begin{bmatrix} 0 \\ 0 \\ |0_n\rangle \\ |w_s\rangle \\ |0_n\rangle \end{bmatrix}, \quad |\lambda_r^{(3)}\rangle = \begin{bmatrix} 0 \\ 0 \\ |0_n\rangle \\ |0_m\rangle \\ |v_r\rangle \end{bmatrix}, \tag{37}$$

where $1 \leq r < n$ and $1 \leq s < m$. Here $L_\pm$, $M_\pm$ and N are normalization factors.

We have the following fidelities:

$$\langle B|e^{-itA_{\mathcal{G}}}|A\rangle = -\sum_{\pm} \frac{e^{-it\lambda_\pm}}{L_\pm^2} + \sum_{\pm} \frac{e^{-it\mu_\pm}}{M_\pm^2} + \frac{1}{N^2}, \tag{38}$$

$$\langle A|e^{-itA_{\mathcal{G}}}|A\rangle = \sum_{\pm} \frac{e^{-it\lambda_\pm}}{L_\pm^2} + \sum_{\pm} \frac{e^{-it\mu_\pm}}{M_\pm^2} + \frac{1}{N^2}. \tag{39}$$

At time $t = 0$, Eq. (39) yields

$$1 = \sum_{\pm} \frac{1}{L_\pm^2} + \sum_{\pm} \frac{1}{M_\pm^2} + \frac{1}{N^2}. \tag{40}$$

So, to achieve perfect state transfer in Eq. (38), we require that

$$e^{-it\lambda_\pm} = -1, \quad e^{-it\mu_\pm} = +1. \tag{41}$$

This implies $t(\tilde{k} \pm \Delta) \in (2\mathbb{Z} + 1)\pi$ and $t(\tilde{k} \pm \Gamma) \in (2\mathbb{Z})\pi$. We restate these conditions as

$$\frac{\tilde{k} \pm \Delta}{\tilde{k} \pm \Gamma} \in \mathbb{Q}_{1,0}, \quad \frac{\tilde{k} \pm \Delta}{\tilde{k} \mp \Gamma} \in \mathbb{Q}_{1,0}. \tag{42}$$

Clearly it is necessary to have $\Delta, \Gamma \in \mathbb{Z}$, else the above quotients are not even rational.

Observe that if both $\tilde{k}$ and n are odd, both quotients lie in $\mathbb{Q}_{1,1}$. If $\tilde{k}$ is even and n is odd, the same is true. If $\tilde{k}$ is odd and n is even, then the numerator and denominator of at least one of the quotients must be congruent to 2 modulo 4, and so one lies in $\mathbb{Q}_{1,1}$. If both $\tilde{k}$ and n are even, then we can divide the numerator and denominator of each quotient by 2 (clearly, then, 4 divides n as well), rewriting the conditions as:

$$\frac{\tilde{k}' \pm \Delta'}{\tilde{k}' \pm \Gamma'} \in \mathbb{Q}_{1,0}, \quad \frac{\tilde{k}' \pm \Delta'}{\tilde{k}' \mp \Gamma'} \in \mathbb{Q}_{1,0}, \tag{43}$$

where $\tilde{k}' = \tilde{k}/2$, $\Delta' = \Delta/2$, and $\Gamma' = \Gamma/2$. Since this is in essence the same set of conditions as before, we argue by infinite descent that there can be no solutions of this form. Since we have ruled out all parity combinations for $\tilde{k}$ and n, there can be no solutions and no perfect state transfer in this case. □
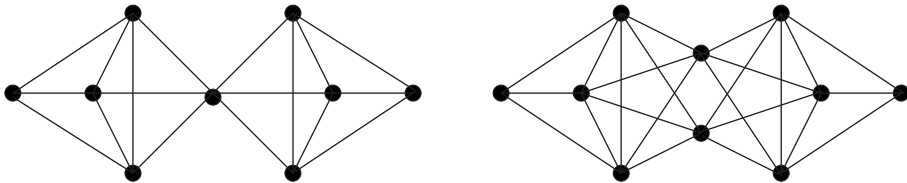

Fig. 7. Cylindrical cones of diameter five with no perfect state transfer (left to right): (a) $K_1 + K_3 + K_1 + K_3 + K_1$; (b) $K_1 + K_3 + \overline{K}_2 + K_3 + K_1$.

5. Equitable Partitions

The path-collapsing argument was used by Christandl *et al.*[7] to show that weighted paths have perfect state transfer. This follows because the (unweighted) n-dimensional hypercube Q_n has perfect state transfer and it can be collapsed to a weighted path. On the other hand, this argument was used in the opposite direction by Childs *et al.*[8] to show that a continuous-time quantum walk on an unweighted layered graph has polynomial hitting time by observing its behavior on a corresponding weighted path.

A natural way to view this reduction is by using equitable distance partitions and their quotient graphs (for example, see Godsil[15] as well as Krovi and Brun[21]). However, most quotient graphs derived this way are directed and hence not suitable for quantum walks. The path-collapsing reduction offers a way to *symmetrize* these directed quotient graphs into undirected graphs. In what follows, we formalize and generalize this argument using the theory of equitable partitions (see Godsil[15]).

Lemma 2. *Let $G = (V, E)$ be a graph with an equitable distance partition $\pi = \uplus_{j=0}^{m-1} V_j$ with respect to vertices a and b. Then, the fidelity of a quantum walk on G between vertices a and b is equivalent to the fidelity of a quantum walk on a symmetrized quotient graph G/π between $\pi(a) = V_0$ and $\pi(b) = V_{m-1}$; namely, if $B_{G/\pi}[j, k] = \sqrt{d_{j,k} d_{k,j}}$, for all $j, k \in [m]$, then*

$$|\langle b | e^{-itA_G} | a \rangle| = |\langle \pi(b) | e^{-itB_{G/\pi}} | \pi(a) \rangle|. \tag{44}$$

Proof. For $j, k \in [m]$, let $d_{j,k}$ be the number of vertices in V_k adjacent to each vertex x in V_j. Let P be the characteristic partition $n \times m$ matrix of π; namely, $P[j, \ell] = 1$ if vertex j belongs to partition V_ℓ, and 0 otherwise. Let Q be the matrix P after we normalize each column; so $Q^T Q = I_n$. Then, we have

$$A_G Q = Q B_{G/\pi}, \tag{45}$$

where

$$B_{G/\pi}[j, k] = \sqrt{d_{j,k} d_{k,j}}. \tag{46}$$

The matrix $B_{G/\pi}$ is defined implicitly in Ref. 7 through the columns of Q (viewed as basis states in a new graph).[a] The following spectral correspondences between A_G and $B_{G/\pi}$ can be shown:

- If $A_G |y\rangle = \lambda |y\rangle$, then $B_{G/\pi} |x\rangle = \lambda |x\rangle$, where $|x\rangle = Q^T |y\rangle$, provided $Q^T |y\rangle \neq 0$.
- If $B_{G/\pi} |x\rangle = \lambda |x\rangle$, then $A_G |y\rangle = \lambda |y\rangle$, where $|y\rangle = Q |x\rangle$.

Suppose that $E(A_G) = \{|y_k\rangle : k \in [n]\}$ is the (orthonormal) set of eigenvectors of A_G; similarly, let $E(B_{G/\pi}) = \{|x_k\rangle : k \in [m]\}$ be the (orthonormal) set of eigenvectors of $B_{G/\pi}$. Since $\pi(a) = \{a\}$ and $\pi(b) = \{b\}$ are singleton partitions, we have $Q^T |a\rangle =$

---

[a]Note $B_{G/\pi}$ is different from $A_{G/\pi}$ (as defined in Ref. 15), since $B_{G/\pi}$ is symmetric and represents an undirected weighted graph whereas $A_{G/\pi}$ represents a directed graph.

$|\pi(a)\rangle$ and $Q^T|b\rangle = |\pi(b)\rangle$. Thus, we have

$$\langle\pi(b)|e^{-itB_{G/\pi}}|\pi(a)\rangle = \langle\pi(b)|\sum_{k=0}^{m-1}(e^{-it\lambda_k}|x_k\rangle\langle x_k|)|\pi(a)\rangle \tag{47}$$

$$= \langle b|\sum_{k=0}^{m-1}(e^{-it\lambda_k}Q|x_k\rangle\langle x_k|Q^T)|a\rangle \tag{48}$$

$$= \langle b|e^{-itA_G}|a\rangle. \tag{49}$$

The last step holds since the orthonormal eigenvectors of A_G can be divided into two types: those that are constant on cells of π (the ones of the form $|y_k\rangle = Q|x_k\rangle$, for some eigenvector $|x_k\rangle$ of $B_{G/\pi}$) and those that sum to zero on each cell of π. The eigenvectors of the latter type do not contribute to the quantum walk between the antipodal vertices a and b. □

Remark. Lemma 2 shows that the double cones $\overline{K}_2 + G$, for regular graphs $G \in \mathcal{G}_{n,k}$, which have diameter two, are *equivalent* (in the sense of the fidelity of quantum walks between the antipodal vertices) to a weighted P_3 with adjacency matrix $\tilde{A}_1$ (shown below).

$$\tilde{A}_1 = \begin{bmatrix} 0 & \sqrt{n} & 0 \\ \sqrt{n} & k & \sqrt{n} \\ 0 & \sqrt{n} & 0 \end{bmatrix}, \quad \tilde{A}_2 = \begin{bmatrix} 0 & \sqrt{n} & 1 \\ \sqrt{n} & k & \sqrt{n} \\ 1 & \sqrt{n} & 0 \end{bmatrix}. \tag{50}$$

The case of the connected double cone $K_2 + G$, where $G \in \mathcal{G}_{n,k}$, can also be shown to be equivalent to the weighted graph with adjacency matrix $\tilde{A}_2$ (shown above). This simplifies the analyses on values of n and k which allows perfect state transfer (see Angeles-Canul *et al.*[12]).

In what follows, we use the generalized path-collapsing argument above to revisit (unweighted) graphs of diameter three and compare them to (weighted) paths of length four. Then, we compare a family of symmetrically weighted paths P_4 (without self-loops) with a construction based on weak products. This symmetry restriction on the weights can be made without loss of generality (see Kay[14]).

Lemma 3. *Let $P_4(\gamma; \kappa)$ denote a weighted path whose middle edge has weight γ while the other two edges have unit weights and whose two internal vertices have self-loops with weight κ each. Let $\Delta_\pm = (1/2)\sqrt{(\kappa \pm \gamma)^2 + 4}$. Then, $P_4(\gamma; \kappa)$ has perfect state transfer if*:

(1) *Case $\kappa \neq 0$: $\Delta_+/\Delta_- \in \mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,0}$ and $\{\gamma/\Delta_+, \gamma/\Delta_-\} \cap (\mathbb{Q}_{0,1} \cup \mathbb{Q}_{1,1}) \neq \emptyset$; or*
(2) *Case $\kappa = 0$: $\{\gamma/\Delta_+, \gamma/\Delta_-\} \subseteq \mathbb{Q}_{1,1}$ or $\{\gamma/\Delta_+, \gamma/\Delta_-\} \subseteq \mathbb{Q}_{1,0}$.*

Proof. Let $k_\pm = (\kappa \pm \gamma)/2$, $\Delta_+^2 = k_+^2 + 1$, and $\Delta_-^2 = k_-^2 + 1$. The adjacency matrix A of $P_4(\gamma; \kappa)$, whose eigenvalues are $\alpha_\pm = k_+ \pm \Delta_+$ and $\beta_\pm = k_- \pm \Delta_-$, and its

corresponding eigenvectors $|\alpha_\pm\rangle$ and $|\beta_\pm\rangle$ are given by:

$$
A = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & \kappa & \gamma & 0 \\ 0 & \gamma & \kappa & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, \quad |\alpha_\pm\rangle = \frac{1}{L_\pm}\begin{bmatrix} 1 \\ 1 \\ \alpha_\pm \\ \alpha_\pm \end{bmatrix}, \quad |\beta_\pm\rangle = \frac{1}{M_\pm}\begin{bmatrix} +1 \\ -1 \\ +\beta_\pm \\ -\beta_\pm \end{bmatrix}, \qquad (51)
$$

where $L_\pm^2 = 4\Delta_+(\Delta_+ \pm k_+)$ and $M_\pm^2 = 4\Delta_-(\Delta_- \pm k_-)$. The end-to-end fidelity of the quantum walk on $P_4(\gamma;\kappa)$ is given by

$$
\langle 3|e^{-itP_4(\gamma;\kappa)}|0\rangle = \sum_\pm \frac{e^{-it\alpha_\pm}}{L_\pm^2} - \sum_\pm \frac{e^{-it\beta_\pm}}{M_\pm^2}. \qquad (52)
$$

At time $t = 0$, $\langle 0|e^{-itP_4(\gamma;\kappa)}|0\rangle$ equals $\sum_\pm 1/L_\pm^2 + \sum_\pm 1/M_\pm^2 = 1$. Thus, to achieve unit fidelity when $\kappa \neq 0$, it suffices to have $e^{-it\gamma/2} = \pm 1$, $\cos(t\Delta_+) = \pm 1$, and $\cos(t\Delta_-) = \mp 1$ where $t\Delta_+$ and $t\Delta_-$ differ in their parities (as a multiple of π) while $t\gamma$ is of even parity. But, when $\kappa = 0$, and thus $\Delta_+ = \Delta_-$, it suffices to simply have $t\gamma$ be of odd parity. □

Note Theorem 4 forms a special case of Lemma 3 when $\kappa \neq 0$. The fact that the analyses are equivalent follows from Lemma 2.

Remark. Let $P_4(\gamma)$ denote $P_4(\gamma;0)$; that is, a weighted path with no self-loops. In this case, $\Delta_+ = \Delta_-$ and a sufficient perfect state transfer condition is $\Delta_+/\gamma \in \mathbb{Q}_{1,1} \cup \mathbb{Q}_{0,1}$. So, $P_4(\gamma)$ has end-to-end perfect state transfer if either:

- for odd integer K and even integer L, with $L > K$, we have $\gamma = 2\sqrt{K^2/(L^2 - K^2)}$; or
- for odd integers K and L, with $2L > K$, we have $\gamma = 2\sqrt{K^2/(4L^2 - K^2)}$.

The weak product $K_2 \times K_{4k}$, for $k \geq 1$, has perfect state transfer by Proposition 1 (see Fig. 4(a)). The path collapsing argument shows $K_2 \times K_{4k}$ is equivalent to $P_4(\tau)$ where $\tau = (4k - 2)/\sqrt{4k - 1} > 1$. Thus, for perfect state transfer, the weak product construction $K_2 \times K_{4k}$ yields edge weights greater than unity, whereas $P_4(\gamma)$ can yield edge weights smaller than unity (with longer PST times). We are not aware of unweighted constructions which can emulate the latter property.

6. Conclusion

Using the Cartesian graph product, Christandl *et al.*[7] constructed two families of perfect state transfer graphs with large diameter, namely, Q_n and $P_3^{\oplus n}$. They also showed that weighted paths have perfect state transfer by a path-collapsing reduction from Q_n. This argument was used specifically on graphs with equitable distance partitions whose cells are empty graphs. Our original motivation was to generalize the Cartesian product construction and extend the path-collapsing argument to larger classes of graphs.

In this work, we described new families of graphs with perfect state transfer using the weak graph product and a generalized lexicographic product (which includes the Cartesian graph product as a special case). We also considered constructions involving double cones, which allow the cell partitions to be non-empty graphs (unlike the Cartesian product graphs). Here, we prove perfect state transfer on double cones of irregular graphs and on double half-cones connected by circulants. These generalized results by Bose *et al.*,[10] Tsomokos,[11] and Angeles-Canul *et al.*[12] on double cones of regular graphs and complement the negative result on double half-cones given by Angeles-Canul *et al.*[13] Although these cone constructions involve small diameter graphs, they provided insights into which intermediate graphs allow antipodal perfect state transfer. Non-antipodal perfect state transfer can also be derived from certain cones (as shown in Angeles-Canul *et al.*[12]).

We also generalized the path-collapsing argument using the theory of equitable partitions. This can be used to show that certain weighted paths with self-loops have perfect state transfer. A possible interesting direction is to study random graphs with equitable distance partitions (as in the Anderson model[22]). A *weighted* path-collapsing argument would also be interesting since it can be used to analyze graphs produced in Feder's intriguing construction.[23] The most elusive graph not covered by this framework is $P_3^{\oplus n}$ since none of the path-collapsing arguments apply. This is because the connections are irregular (see Fig. 1(b)). We leave these as open questions.

Acknowledgments

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