Perfect quantum state transfer using Hadamard diagonalizable graphs

Nathaniel Johnston\textsuperscript{a,b}, Steve Kirkland\textsuperscript{c}, Sarah Plosker\textsuperscript{b,c,d}, Rebecca Storey\textsuperscript{d}, Xiaohong Zhang\textsuperscript{c}

\textsuperscript{a}Department of Mathematics \& Computer Science, Mount Allison University, Sackville, NB, Canada E4L 1E4
\textsuperscript{b}Department of Mathematics \& Statistics, University of Guelph, Guelph, ON, Canada N1G 2W1
\textsuperscript{c}Department of Mathematics, University of Manitoba, Winnipeg, MB, Canada R3T 2N2
\textsuperscript{d}Department of Mathematics \& Computer Science, Brandon University, Brandon, MB, Canada R7A 6A9

Abstract

Quantum state transfer within a quantum computer can be achieved by using a network of qubits, and such a network can be modelled mathematically by a graph. Here, we focus on the corresponding Laplacian matrix, and those graphs for which the Laplacian can be diagonalized by a Hadamard matrix. We give a simple eigenvalue characterization for when such a graph has perfect state transfer at time $\pi/2$; this characterization allows one to choose the correct eigenvalues to build graphs having perfect state transfer. We characterize the graphs that are diagonalizable by the standard Hadamard matrix, showing a direct relationship to cubelike graphs. We then give a number of constructions producing a wide variety of new graphs that exhibit perfect state transfer, and we consider several corollaries in the settings of both weighted and unweighted graphs, as well as how our results relate to the notion of pretty good state transfer. Finally, we give an optimality result, showing that among regular graphs of degree at most 4, the hypercube is the sparsest Hadamard diagonalizable connected unweighted graph with perfect state transfer.

Keywords: Laplacian matrix, Hadamard diagonalizable graph, quantum state transfer, cubelike graphs, double cover, perfect state transfer

2010 MSC: 05C50, 05C76, 15A18, 81P45

Email address: ploskers@brandonu.ca (Sarah Plosker)
1. Introduction

Accurate transmission of quantum states between processors and/or registers of a quantum computer is critical for short distance communication in a physical quantum computing scheme. Bose [8] first proposed the use of spin chains to accomplish this task over a decade ago. Since then, much work has been done on perfect state transfer (PST), which accomplishes this task perfectly in the sense that the state read out by the receiver at some time $t_0$ is, with probability equal to one, identical up to complex modulus to the input state of the sender at time $t = 0$.

Many families of graphs have been found to exhibit PST, including the join of a weighted two-vertex graph with any regular graph [2], Hamming graphs [2] (see also [7, 12, 13]), a family of double-cone non-periodic graphs [3], and a family of integral circulant graphs [6] (see also [3]). It is easy to see that the Cartesian product of two graphs having PST at the same time also has PST [1, Sec. 3.3]. Much work has also been done with respect to analyzing the sensitivity [10, 15, 16, 17, 20, 21, 23], or even correcting errors [19], of quantum spin systems. Signed graphs and graphs with arbitrary edge weights have also been considered (see [9] and the references therein), due to the intriguing fact that certain graphs that do not exhibit PST when unsigned/unweighted can exhibit PST when signed or weighted properly. Three articles particularly relevant to the work herein are [7, 11], which characterized perfect state transfer in cubelike graphs, a family of graphs that are Hadamard diagonalizable, and [14], which shows that perfect state transfer occurs in graphs constructed in a manner similar to our merge operation, called the “$\times$” operation.

The general approach taken in the literature is to model a quantum spin system with an undirected connected graph, where the dynamics of the system are governed by the Hamiltonian of the system: for $XX$ dynamics the Hamiltonian is the adjacency matrix corresponding to the graph, and for Heisenberg ($XXX$) dynamics the Hamiltonian is the Laplacian matrix corresponding to the graph. In the case of $XXX$ dynamics (on which we focus exclusively in this paper), there is more structure to work with since we know that the smallest eigenvalue of a Laplacian matrix is zero, with corresponding eigenvector 1 (the all-ones vector). We note in passing that in the case of regular graphs (which we deal with frequently in this paper), presence or absence of PST is identical under $XX$ dynamics and $XXX$ dynamics.

Our contribution to the theory of perfect state transfer is to characterize graphs that are diagonalizable by the standard Hadamard matrix, connecting this property with the notion of cubelike graphs, and to detail procedures for creating new
graphs with PST.

Our focus on graphs having a Hadamard diagonalizable Laplacian is not as restrictive as it might seem at first glance; Hadamard matrices are ubiquitous in quantum information theory, and because of the special structure of Hadamard matrices the corresponding graphs tend to exhibit a good deal of symmetry. As a result, many of the known graphs with PST are actually Hadamard diagonalizable, such as the hypercube. Furthermore, integer-weighted graphs with Hadamard diagonalizable Laplacian are convenient to work with in our setting because they are known to be regular, with spectra consisting of even integers (see [5] and Theorem 2 below); consequently the corresponding graph often exhibits PST between two of its vertices at time $t_0 = \pi/2$ (see Theorem 3 for a more specific statement).

In Section 2, we give a quick review of the graph theory and quantum state transfer definitions and tools that we will use. In Section 3 we give an eigenvalue characterization connecting a graph being Hadamard diagonalizable and it having PST at time $\pi/2$ between two of its vertices. We further give a connection between diagonalizability by the standard Hadamard matrix and cubelike graphs, completely characterizing such graphs. In Section 4, we describe several ways to construct new Hadamard diagonalizable graphs from old ones, including our “merge” operation, a weighted variant of the “$\times$” operation, which takes two Hadamard diagonalizable graphs as input, and produces a new (larger) Hadamard diagonalizable graph with PST as output under a wide variety of conditions. We also present several results demonstrating the usefulness of this operation and the types of graphs with PST that it can produce. In Section 5 we discuss how our results generalize to graphs with non-integer edge weights, which involves the notion of pretty good state transfer (PGST), and we close in Section 6 with some results concerning the optimality in terms of timing errors and manufacturing errors of Hadamard diagonalizable graphs.

2. Preliminaries

2.1. Graph Theory Basics

For a weighted undirected graph $G$ on $n$ vertices, its corresponding $n \times n$ adjacency matrix $A = (a_{jk})$ is defined by

$$a_{jk} = \begin{cases} w_{j,k} & \text{if } j \text{ and } k \text{ are adjacent} \\ 0 & \text{otherwise,} \end{cases}$$

where $w_{j,k}$ is the weight of the edge between vertices $j$ and $k$. Its corresponding $n \times n$ Laplacian matrix is defined by $L = D - A$, where $D$ is the diagonal matrix
of row sums of $A$, known as the degree matrix associated to $G$. Often $w_{j,k}$ in the above is taken to be 1 for all adjacent $j,k$, in which case the graph is said to be unweighted. A signed graph is a graph for which the non-zero weights can be either $\pm 1$. A weighted graph is a graph for which there is no restriction on $w_{j,k}$ (although the weights are typically taken to be in $\mathbb{R}$, as they are in this paper).

An unweighted graph $G$ is regular if each of its vertices has the same number of neighbours, or, more specifically, $k$-regular if each of its vertices has exactly $k$ adjacent neighbours. The weighted analogue of a regular graph is a graph where the sum of all the weights of edges incident with a particular vertex is the same for all vertices. We will be interested in weighted graphs with this equal “weighted degree” property; for simplicity, we simply call this the degree of the graph. A graph is connected if there is a path (a sequence of edges connecting a sequence of vertices) between every pair of distinct vertices and complete if there is an edge between every pair of distinct vertices (the complete graph on $n$ vertices is denoted $K_n$).

There are several different operations that can be performed to turn two graphs into a new (typically larger) graph. Specifically, given graphs $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$, where $V_1$ and $E_1$ are the set of all vertices and the set of all edges, respectively, in the graph $G_1$ (and similarly for $V_2$ and $E_2$), then

1. The union of $G_1$ and $G_2$ is the graph $G_1 + G_2 = (V_1 \cup V_2, E_1 \cup E_2)$;

2. The join of $G_1$ and $G_2$ is the graph $G_1 \vee G_2 = (G_1^c + G_2^c)^c$ where every vertex of $G_1$ is connected to every vertex of $G_2$, and all of the original edges of $G_1$ and $G_2$ are retained as well;

3. The Cartesian product of $G_1$ and $G_2$ is the graph $G_1 \square G_2 = (V_1 \times V_2, E_3)$ where $V_1 \times V_2$ is the cartesian product of the two original sets of vertices, and there is an edge in $G_1 \square G_2$ between vertices $(g_1, g_2)$ and $(h_1, h_2)$ if and only if either (i) $g_1 = h_1$ and there is an edge between $g_2$ and $h_2$ in $G_2$, or (ii) $g_2 = h_2$ and there is an edge between $g_1$ and $h_1$ in $G_1$.

One can also define the Cartesian product of weighted graphs $G_1$ and $G_2$ by defining (i) the weight of the edges between $(g_1, g_2)$ and $(h_1, h_2)$ in $G_1 \square G_2$ to be the same as the weight between $g_2$ and $h_2$ in $G_2$, and (ii) the weight of the edges between $(g_1, g_2)$ and $(h_1, g_2)$ in $G_1 \square G_2$ to be the same as the weight between $g_1$ and $h_1$ in $G_1$; and

4. If $V_1 = V_2$, let $G_1 \ltimes G_2$ be the graph defined by the adjacency matrix

$$A(G_1 \ltimes G_2) = \begin{bmatrix} A(G_1) & A(G_2) \\ A(G_2) & A(G_1) \end{bmatrix},$$

where $A(\cdot)$ is the adjacency matrix of the given graph. If the edge sets of $G_1$ and $G_2$ are disjoint, then $G_1 \ltimes G_2$ is a double cover of the graph with adjacency matrix $A(G_1) + A(G_2)$. 

4
We recall that a Hadamard matrix (or simply, a Hadamard) of order \( n \) is an \( n \times n \) matrix \( H \) with entries \( +1 \) and \( -1 \), such that \( HH^T = nI \). Let \( H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, H_2 = \begin{bmatrix} H_1 & H_1 \\ H_1 & -H_1 \end{bmatrix}, \ldots, H_n = \begin{bmatrix} H_{n-1} & H_{n-1} \\ H_{n-1} & -H_{n-1} \end{bmatrix} \). This construction gives the standard Hadamards of order \( 2^n \). The results herein may be of use in the physical setting because Hadamards are among the simplest non-trivial gates to implement in the lab (the standard \( n \)-qubit Hadamard with a scaling factor of \( 1/2^{n/2} \) is frequently used in quantum information theory). From the definition of a Hadamard matrix, it is clear that any two rows of \( H \) are orthogonal, and any two columns of \( H \) are also orthogonal. This property does not change if we permute rows or columns or if we multiply some rows or columns by \( -1 \). This leads to the simple but important observation that, given a Hadamard matrix, it is always possible to permute and sign its rows and columns so that all entries of the first row and all entries of the first column are all \( 1 \)'s. A Hadamard matrix in this form is said to be normalized [5]. Given a graph \( G \) on \( n \) vertices with corresponding Laplacian matrix \( L \), if we can write \( L = \frac{1}{n}HAH^T \) for some Hadamard \( H \) and diagonal matrix \( \Lambda \), then we say that \( G \) (or, that \( L \)) is Hadamard diagonalizable. If \( G \) is Hadamard diagonalizable by some Hadamard \( H \), then \( G \) is also Hadamard diagonalizable by a corresponding normalized Hadamard [5, Lemma 4]. Thus, there is no loss of generality in assuming that a Hadamard diagonalizable graph is in fact diagonalized by a normalized Hadamard matrix. Note that “normalized” in this setting does not imply scaling \( H \) to satisfy \( \| H \| = 1 \).

2.2. Perfect state transfer basics

A graph exhibits perfect state transfer (PST) at time \( t_0 \) if \( p(t_0) := |e_j^T e^{it_0H} e_k|^2 = 1 \) for some vertices \( j \neq k \) and some time \( t_0 > 0 \), where \( \mathcal{H} \) is the Hamiltonian of the system (either the adjacency matrix \( A \) or the Laplacian matrix \( L \), depending on the system’s dynamics). In other words, the graph has perfect state transfer if and only if \( e^{it_0H} e_k \) is a scalar multiple of \( e_j \) (or, equivalently, if \( e^{it_0H} e_j \) is a scalar multiple of \( e_k \)). Typically we say that a graph has PST from vertex \( j \) to vertex \( k \) if it exhibits PST for some vertices \( j \) and \( k \) and \( j < k \).

A slightly weaker property is that of pretty good state transfer (PGST): a graph exhibits PGST (for some vertices \( j \neq k \)) if for every \( \varepsilon > 0 \), there exists a time \( t_\varepsilon \) such that \( p(t_\varepsilon) := |e_j^T e^{it_\varepsilon H} e_k|^2 \geq 1 - \varepsilon \).

The following observation is well-known.

**Remark 1.** For a general integer-weighted graph \( G \), assume that \( a \) is the greatest common divisor of all the edge weights of \( G \) and that \( L \) is the Laplacian matrix...
of $G$. Let $G'$ denote the integer-weighted graph with Laplacian $1/a L$. Since $e^{itaL} = e^{ita(\frac{1}{a} L)}$ for all $t$, we find that $G$ has PST at $\pi/(2a)$ if and only if $G'$ has PST at $\pi/2$. This allows us to identify more graphs having PST: for example, if $G$ has PST at $\pi/2$, and we are given the graph with Laplacian matrix $2L$, we know that it has PST at $\pi/4$.

2.3. Cubelike graphs

A large family of graphs, of which the hypercube is a member, is the family of cubelike graphs [7, 11]: Take a set $C \subset \mathbb{Z}^d_2 = \mathbb{Z}_2 \times \cdots \times \mathbb{Z}_2$ ($d$ times), where $C$ does not contain the all-zeros vector. Construct the cubelike graph $G(C)$ with vertex set $V = \mathbb{Z}^d_2$ and two elements of $V$ are adjacent if and only if their difference is in $C$. The set $C$ is called the connection set of the graph $G(C)$. The following result characterizes PST at $\pi/2$ for cubelike graphs.

Theorem 1. [7, Theorem 1], [11, Theorem 2.3] Let $C$ be a subset of $\mathbb{Z}^d_2$ and let $\sigma$ be the sum of the elements of $C$. If $\sigma \neq 0$, then PST occurs in $G(C)$ from $j$ to $j + \sigma$ at time $\pi/2$. If $\sigma = 0$, then $G(C)$ is periodic with period $\pi/2$ (every vertex has perfect state transfer with itself at time $t_0 = \pi/2$).

The code of $G(C)$ is the row space of the $d \times |C|$ matrix $M$ constructed by taking the elements of $C$ as its columns. When the sum of the elements of $C$ is zero, it has been shown [11] that if perfect state transfer occurs on a cubelike graph, then it must take place at time $\pi/2D$, where $D$ is the greatest common divisor of the (Hamming) weights of the binary strings in the code.

3. Hadamard diagonalizable graphs with PST

The following theorem originally appeared in [5], restricted to the case of unweighted graphs. The version below allows for arbitrary integer edge weights. Although its proof is almost identical to its unweighted version, we include it here for completeness.

Theorem 2. [5, Theorem 5] If $G$ is an integer-weighted graph that is Hadamard diagonalizable, then $G$ is regular and all the eigenvalues of its Laplacian are even integers.

Proof. Without loss of generality we assume that the Laplacian matrix for $G$ is diagonalized by a normalized Hadamard matrix; observe then that the first column of that Hadamard is the all-ones vector, and that it corresponds to the eigenvalue
Choose a non-zero eigenvalue \( \lambda \) of the Laplacian matrix \( L \) associated to \( G \); the corresponding column of the Hadamard matrix that diagonalizes \( L \) is an eigenvector corresponding to \( \lambda \). One can split the graph \( G \) into two subgraphs, \( G_1 \) and \( G_2 \) (with Laplacians \( L_1 \) and \( L_2 \)), corresponding to the \( n/2 \) entries of 1 and the \( n/2 \) entries of \(-1\) of the eigenvector corresponding to \( \lambda \). By applying a permutation similarity if necessary, we find that

\[
\begin{bmatrix}
L_1 + X_1 & -R \\
-R^T & L_2 + X_2
\end{bmatrix}
\begin{bmatrix}
1 \\
-1
\end{bmatrix}
= \lambda
\begin{bmatrix}
1 \\
-1
\end{bmatrix},
\]

for some matrices \( X_1 \), \( X_2 \), and \( R \). Necessarily \( X_1 \), \( X_2 \) are diagonal, and note that we have \( X_1 1 = R1 \) and \( X_2 1 = R^T 1 \).

Since \( \lambda 1 = L_1 1 + X_1 1 + R1 = 2X_1 1 \), and since \( G \) is integer-weighted, we deduce that \( \lambda \) is an even integer. Hence each eigenvalue of the Laplacian is an even integer.

Next we show that \( G \) is regular. For concreteness, suppose that \( G \) has \( n \) vertices and that \( H \) is a normalized Hadamard matrix so that \( LH = HD \) for some diagonal matrix \( D \). Fix an index \( j \) between 1 and \( n \), and let \( S_j \) be the diagonal matrix with diagonal entries \( \pm 1 \) such that \( e_j^T HS_j = 1^T \). Observe that \( LHS_j = HS_j D \), and that \( HS_j \) is also a Hadamard matrix. Since the \( j \)-th row of \( HS_j \) is the all-ones vector and the remaining rows are orthogonal to it, we deduce that \( HS_j 1 = ne_j \). Consequently, \( e_j^T LHS_j 1 = ne_j^T L e_j \). On the one hand, we have \( e_j^T LHS_j 1 = e_j^T HS_j D 1 = 1^T D 1 \). Thus, for each \( j = 1, \ldots, n \), \( e_j^T L e_j = \frac{1}{n} 1^T D 1 \), so \( G \) is regular, as desired.

For an integer-weighted graph that is diagonalizable by some Hadamard matrix, we now give a precise characterization of its eigenvalues when it exhibits PST at time \( t_0 = \pi/2 \). The proof applies a standard characterization of PST; see [18], for example.

**Theorem 3.** Let \( G \) be an integer-weighted graph that is Hadamard diagonalizable by a Hadamard of order \( n \). Let \( H = (h_{uv}) \) be a corresponding normalized Hadamard. Denote the eigenvalues of the Laplacian matrix \( L \) corresponding to \( G \) by \( \lambda_1, \ldots, \lambda_n \), so that \( LH e_j = \lambda_j H e_j \), \( j = 1, \ldots, n \). Then \( G \) has PST from vertex \( j \) to vertex \( k \) at time \( t_0 = \pi/2 \) if and only if for each \( \ell = 1, \ldots, n \), \( \lambda_\ell \equiv 1 - h_{j\ell} h_{k\ell} \mod 4 \).

**Proof.** Let \( \Lambda \) be the diagonal matrix of eigenvalues such that \( L = \frac{1}{n} H \Lambda H^T \), and hence \( e^{i(\pi/2)L} = \frac{1}{n} H e^{i(\pi/2)H} H^T \). By the definition of PST, it follows that \( G \) has
PST from vertex $j$ to vertex $k$ at $t_0 = \pi/2$ if and only if $e^{i(\pi/2)\Lambda}H^T e_j$ is a scalar multiple of $H^T e_k$. Since the first column of $H$ is the all ones vector $1$, i.e. an eigenvector of $L$ corresponding to the eigenvalue 0, we know that the first entry of $e^{i(\pi/2)\Lambda}H^T e_j$ is $h_{j1} = 1$, and the first entry of $H^T e_k = h_{k1} = 1$. Thus we deduce that not only is $e^{i(\pi/2)\Lambda}H^T e_j$ a scalar multiple of $H^T e_k$, but that the multiple must be 1, i.e., we have PST from vertex $j$ to $k$ at $\pi/2$ if and only if

$$e^{i(\pi/2)\Lambda}H^T e_j = H^T e_k.$$  \hfill (1)

Note that

$$e^{i(\pi/2)\lambda_\ell} = \begin{cases} 1 & \text{if } \lambda_\ell \equiv 0 \mod 4 \\ -1 & \text{if } \lambda_\ell \equiv 2 \mod 4. \end{cases}$$

Consequently, (1) holds if and only if, for each $\ell = 1, \ldots, n$, if $h_{j\ell}h_{k\ell} = 1$ then $\lambda_\ell \equiv 0 \mod 4$, and if $h_{j\ell}h_{k\ell} = -1$ then $\lambda_\ell \equiv 2 \mod 4$. The conclusion follows. \qed

It is worth noting that Theorem 3 already gives an extremely easy method for creating weighted Hadamard diagonalizable graphs exhibiting PST, since for any normalized Hadamard matrix $H$ we can choose the eigenvalues in $\Lambda$ to satisfy the required mod 4 equation, and then $L = \frac{1}{n}H\Lambda H^T$ will necessarily be the Laplacian of some rational-weighted graph with PST at time $t_0 = \pi/2$ (the graph will be integer-weighted provided $n$ divides each edge weight in this construction).

It is known that the adjacency matrix of any cubelike graph is diagonalized by the standard Hadamard matrix (see [7]). The following result provides the converse; in the proof, it will be convenient to denote the graph (possibly containing loops) with adjacency matrix $A$ by $\Gamma(A)$.

**Lemma 1.** Suppose that $k \in \mathbb{N}$ and that $A$ is a symmetric $(0,1)$ matrix that is diagonalizable by the standard Hadamard matrix of order $2^k$. Then

1. $A$ has constant diagonal;
2. if $A$ has zero diagonal then it is the adjacency matrix of a cubelike graph;
3. if $A$ has all ones on the diagonal, then $A - I$ is the adjacency matrix of a cubelike graph.

**Proof.** We proceed by induction on $k$. For $k = 1$, it is straightforward to see that the $(0,1)$ symmetric matrices that are diagonalized by $H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ are:
\[
\begin{bmatrix}
0 & 0 \\
0 & 0 \\
1 & 0 \\
0 & 1 \\
1 & 1 \\
\end{bmatrix}, \begin{bmatrix}
1 & 0 \\
0 & 1 \\
1 & 0 \\
1 & 1 \\
\end{bmatrix}.
\]
For these matrices, conclusions (1)–(3) follow readily.

Suppose that the result holds for some \(k \in \mathbb{N}\) and that \(A\) is of order \(2^{k+1}\). Write the standard Hadamard matrix of order \(2^{k+1}\) as
\[
H_{k+1} = \begin{bmatrix}
H_k & H_k \\
H_k & -H_k
\end{bmatrix},
\]
where \(H_k\) is the standard Hadamard matrix of order \(2^k\). Partition \(A\) accordingly as
\[
\begin{bmatrix}
A_1 & X \\
X^T & A_2
\end{bmatrix}.
\]
Then there are diagonal matrices \(D_1, D_2\) such that
\[
\begin{bmatrix}
H_k & H_k \\
H_k & -H_k
\end{bmatrix} \begin{bmatrix}
A_1 & X \\
X^T & A_2
\end{bmatrix} \begin{bmatrix}
H_k & H_k \\
H_k & -H_k
\end{bmatrix} = \begin{bmatrix}
D_1 & O \\
O & D_2
\end{bmatrix}.
\]
Hence
\[
\begin{bmatrix}
H_k(A_1 + A_2 + X + X^T)H_k & H_k(A_1 - A_2 - X + X^T)H_k \\
H_k(A_1 - A_2 + X - X^T)H_k & H_k(A_1 + A_2 - X - X^T)H_k
\end{bmatrix} = \begin{bmatrix}
D_1 & O \\
O & D_2
\end{bmatrix}.
\]
We deduce that \(A_1 - A_2 = X - X^T\); since \(A_1 - A_2\) is symmetric and \(X - X^T\) is skew-symmetric, it must be the case that \(A_1 = A_2\) and \(X = X^T\). Then \(H_k\) diagonalizes both \(2(A_1 + X)\) and \(2(A_1 - X)\), and we conclude that \(H_k\) diagonalizes \(A_1\) and diagonalizes \(X\). In particular the induction hypothesis applies to \(A_1\) and \(X\). Thus \(A_1\) has constant diagonal, and hence so does \(A\).

Suppose that \(A\) has zero diagonal. Applying the induction hypothesis to \(A_1\), we find that \(\Gamma(A_1)\) is cubelike. Let \(C_1\) denote its connection set. Applying the induction hypothesis to \(X\), then either \(X\) has zero diagonal and so that \(\Gamma(X)\) is a cubelike graph with connection set \(C_2\), say, or \(\Gamma(X - I)\) is a cubelike graph with connection set \(\tilde{C}_2\). Set \(C_2 = \tilde{C}_2 \cup \{0\}\).

We label the vertices of the graph \(\Gamma(A)\) with vectors in \(\mathbb{Z}_2^{k+1}\) in increasing order if considered as binary numbers. So the first \(2^k\) rows/columns of \(A\) are labelled as \(\begin{bmatrix} 0 \\ z \end{bmatrix}\), where \(z \in \mathbb{Z}_2^k\), and the last \(2^k\) rows/columns of \(A\) are of labelled as \(\begin{bmatrix} 1 \\ z \end{bmatrix}\), where \(z \in \mathbb{Z}_2^k\). Now construct the following connection set:
\[
C = \left\{\begin{bmatrix} 0 \\ x \end{bmatrix}, x \in C_1\right\} \cup \left\{\begin{bmatrix} 1 \\ y \end{bmatrix}, y \in C_2\right\}.
\]
It follows that \(A\) is the adjacency matrix of the cubelike graph with connection set \(C\).
If $A$ has all ones on the diagonal we proceed as above with $A - I$.
This establishes the induction steps for (1)--(3). □

**Corollary 1.** Let $G$ be an unweighted graph with Laplacian matrix $L$. Then $L$ is diagonalized by the standard Hadamard matrix if and only if $G$ is a cubelike graph.

**Proof.** If $L$ is diagonalized by the standard Hadamard matrix, then in particular $G$ is regular by Theorem 2. Hence the adjacency matrix of $G$ is diagonalized by the standard Hadamard matrix, so by Lemma 1, $G$ is cubelike. Conversely, if $G$ is cubelike, it is regular and its adjacency matrix is diagonalized by the standard Hadamard matrix. We now deduce that $L$ is diagonalized by the standard Hadamard matrix. □

4. Creation of new Hadamard diagonalizable graphs with PST

It is known that the union of a PST graph with itself still exhibits PST. Here, we show that for a graph $G$ on $n \geq 4$ vertices that is diagonalizable by some Hadamard matrix and that has PST at time $\pi/2$, both its complement and the join of $G$ with itself are Hadamard diagonalizable and have PST at time $t_0 = \pi/2$.

**Proposition 1.** Let $G$ be an integer-weighted graph on $n \geq 4$ vertices that is diagonalizable by a Hadamard matrix $H$, and that has perfect state transfer from vertex $j$ to vertex $k$ at time $t_0 = \pi/2$. Then its complement $G^c$ is also diagonalizable by $H$, and has the same PST pairs and PST time as $G$. Furthermore, the join $G \lor G$ of $G$ with itself is diagonalizable by the Hadamard matrix $\begin{bmatrix} H & H \\ H & -H \end{bmatrix}$, and has PST from vertex $j$ to vertex $k$ at time $t_0 = \pi/2$.

**Proof.** Without loss of generality we can assume that $H$ is a normalized Hadamard matrix. The result that $G^c$ and $G \lor G$ are diagonalizable follows from Lemma 7 in [5]. If we denote the eigenvalues of the Laplacian of $G$ by $\lambda_1 = 0, \lambda_2, \ldots, \lambda_n$, then from Theorem 3 we know that for $\ell = 1, \ldots, n$, $\lambda_\ell \equiv 1 - h_{jj}h_{kk} \mod 4$. Therefore the eigenvalues $0, n - \lambda_2, \ldots, n - \lambda_n$ of $G^c$ satisfy $(n - \lambda_\ell) \equiv -(1 - h_{jj}h_{kk}) \equiv 1 - h_{jj}h_{kk} \mod 4$, since $1 - h_{jj}h_{kk}$ is either 0 or 2 mod 4 and $n$ must be a multiple of 4 in order for a Hadamard of order $n$ to exist.

Again from Theorem 3 we then know that $G^c$ has PST from vertex $j$ to $k$ at time $\pi/2$. Thus $G \lor G = (G^c + G^c)^c$ also has PST from vertex $j$ to $k$ at time $\pi/2$. □
Note that we can also prove that $G^c$ exhibits PST at $t_0 = \pi/2$ by noticing that if $\lambda$ is a nonzero Laplacian eigenvalue for $G$, then $n - \lambda$ is a Laplacian eigenvalue for $G^c$ with the same eigenvector. As $n - \lambda \equiv \lambda \mod 4$, the conclusion now follows from Theorem 3.

We now introduce a modification of $G_1 \ltimes G_2$ that, much like $G_1 \ltimes G_2$, can be used to construct new graphs with PST from old ones. Suppose that $G_1$ and $G_2$ are two weighted graphs of order $n$, with Laplacians $L_1 = D_1 - A_1$ and $L_2 = D_2 - A_2$, respectively. Then we define the merge of $G_1$ and $G_2$ with respect to the weights $w_1$ and $w_2$ to be the graph $G_{1 \odot w_1 \circ w_2} G_2$ with Laplacian

$$
\begin{bmatrix}
w_1 L_1 + w_2 D_2 & -w_2 A_2 \\
-w_2 A_2 & w_1 L_1 + w_2 D_2
\end{bmatrix}.
$$

In the case that $w_1 = w_2 = 1$, we denote the merge simply by $G_1 \circ G_2$, and it recovers $G_1 \ltimes G_2$.

![Figure 1](image)

Figure 1: A depiction of two Hadamard diagonalizable graphs (left) and their merge (right). The new graph has two copies of the original vertex set, and there is an edge $(j, k)$ and $(n + j, n + k)$ if and only if $G_1$ (top left) had edge $(j, k)$, and there is an edge $(j, n + k)$ and only if $G_2$ (bottom left) had edge $(j, k)$.

Observe that if $G_1$ and $G_2$ are both diagonalizable by the same Hadamard matrix $H$, then $G_{1 \odot w_1 \circ w_2} G_2$ is also Hadamard diagonalizable, by the matrix
\[ \begin{bmatrix} H & H \\ H & -H \end{bmatrix} \]; this observation is what motivates our definition of the merge. While this operation is a bit less intuitive than the other ones we saw, it does have an interpretation in terms of the vertices and edges of the original graphs. Specifically, if \( G_1 \) and \( G_2 \) each have vertices labelled \( \{1, \ldots, n\} \), then \( G_1 \odot w_1 \odot w_2 G_2 \) has twice as many vertices, which we label \( \{1, \ldots, 2n\} \). Furthermore, if \( G_1 \) has edge \( (j, k) \) with weight \( w_{jk} \) then \( G_1 \odot w_1 \odot w_2 G_2 \) has edges \( (j, k) \) and \( (n + j, n + k) \), each with weight \( w_1 w_{jk} \). Similarly, if \( G_2 \) has edge \( (j, k) \) with weight \( w_{jk} \) then \( G_1 \odot w_1 \odot w_2 G_2 \) has edge \( (j, n + k) \) and \( (k, n + j) \) with weight \( w_2 w_{jk} \). See Fig. 1 for an example in the unweighted case—the Laplacian matrices corresponding to \( G_1 \), \( G_2 \), and \( G_1 \odot G_2 \) in the example are, respectively,

\[
L_1 = \begin{bmatrix}
2 & -1 & 0 & -1 \\
-1 & 2 & -1 & 0 \\
0 & -1 & 2 & -1 \\
-1 & 0 & -1 & 2
\end{bmatrix}, \quad L_2 = \begin{bmatrix}
2 & -1 & -1 & 0 \\
-1 & 2 & 0 & -1 \\
-1 & 0 & 2 & -1 \\
0 & -1 & -1 & 2
\end{bmatrix}, \quad \text{and}
\]

\[
L_3 = \begin{bmatrix}
4 & -1 & 0 & -1 & 0 & -1 & 0 \\
-1 & 4 & -1 & 0 & -1 & 0 & -1 \\
0 & -1 & 4 & -1 & 0 & -1 \\
-1 & 0 & -1 & 4 & 0 & -1 & 0 \\
0 & -1 & -1 & 0 & 4 & -1 & 0 \\
-1 & 0 & 0 & -1 & -1 & 4 & -1 \\
-1 & 0 & 0 & -1 & 0 & -1 & 4
\end{bmatrix}.
\]

We now describe an exact characterization of when the merge of two integer-weighted graphs which are diagonalizable by the same Hadamard matrix has PST at time \( t_0 = \pi/2 \). This gives us a wide variety of new graphs with PST; in particular, the merge operation produces perfect state transfer graphs in a variety of scenarios. We note that the result below can be proven by using techniques developed in [14] for the adjacency matrix. However for completeness, we give a separate proof that relies on Theorem 3.

**Theorem 4.** Suppose \( G_1 \) and \( G_2 \) are integer-weighted graphs on \( n \) vertices, both of which are diagonalizable by the same Hadamard matrix \( H \). Fix \( w_1, w_2 \in \mathbb{Z} \) and let \( L_1 = d_1 I - A_1 \), \( L_2 = d_2 I - A_2 \) be the Laplacian matrices for \( G_1, G_2 \), respectively. Then \( G_1 \odot w_1 \odot w_2 G_2 \) has PST from vertex \( p \) to \( q \), where \( p < q \), at time \( t_0 = \pi/2 \) if and only if one of the following 8 conditions holds:
1. \( p, q \in \{1, \ldots, n\} \) and
   (a) \( w_1 \) is odd, \( w_2 \) is even, and \( G_1 \) has PST from \( p \) to \( q \) at \( t_0 = \pi/2 \), or
   (b) \( w_1 \) and \( d_2 \) are even, \( w_2 \) is odd, and \( G_2 \) has PST from \( p \) to \( q \) at \( t_0 = \pi/2 \), or
   (c) \( w_1 \) and \( w_2 \) are odd, \( d_2 \) is even, and the weighted graph with Laplacian \( L_1 + L_2 \) has PST from \( p \) to \( q \) at \( t_0 = \pi/2 \);

2. \( p, q \in \{n + 1, \ldots, 2n\} \) and
   (a) \( w_1 \) is odd, \( w_2 \) is even, and \( G_1 \) has PST from \( p - n \) to \( q - n \) at \( t_0 = \pi/2 \), or
   (b) \( w_1 \) and \( d_2 \) are even, \( w_2 \) is odd, and \( G_2 \) has PST from \( p - n \) to \( q - n \) at \( t_0 = \pi/2 \), or
   (c) \( w_1 \) and \( w_2 \) are odd, \( d_2 \) is even, and the weighted graph with Laplacian \( L_1 + L_2 \) has PST from \( p - n \) to \( q - n \) at \( t_0 = \pi/2 \);

3. \( p \in \{1, \ldots, n\} \), \( q \in \{n + 1, \ldots, 2n\} \) and
   (a) \( w_1 \) is even, \( w_2 \) and \( d_2 \) are odd, and \( G_2 \) has PST from \( p \) to \( q - n \) at \( t_0 = \pi/2 \), or
   (b) \( w_1, w_2, \) and \( d_2 \) are all odd, and the weighted graph with Laplacian matrix \( L_1 + L_2 \) has PST from \( p \) to \( q - n \) at \( t_0 = \pi/2 \).

**Proof.** Without loss of generality we can assume that \( H \) is a normalized Hadamard matrix. Denote the diagonal matrices of eigenvalues for \( L_1, L_2 \) by \( \Lambda_1, \Lambda_2 \), respectively, so that \( L_j = \frac{1}{n} H \Lambda_j H^T \), \( j = 1, 2 \). Then the Laplacian of \( G_1 \) \( w_1 \cap w_2 \) \( G_2 \) is
\[
L_3 = \begin{bmatrix}
w_1 L_1 + w_2 d_2 I & -w_2 A_2 \\
-w_2 A_2 & w_1 L_1 + w_2 d_2 I
\end{bmatrix}.
\]
Further,
\[
L_3 = \frac{1}{2n} \begin{bmatrix}
H & H \\
H & -H
\end{bmatrix} \begin{bmatrix}w_1 \Lambda_1 + w_2 \Lambda_2 & 0 \\
0 & w_1 \Lambda_1 - w_2 \Lambda_2 + 2w_2 d_2 I
\end{bmatrix} \begin{bmatrix}H & H \\
H & -H
\end{bmatrix}^T.
\]
Denote the eigenvalues of \( L_1, L_2 \) by \( \lambda^{(1)}_{\ell}, \lambda^{(2)}_{\ell} \), \( \ell = 1, \ldots, n \), respectively.

1. Suppose that \( p, q \in \{1, \ldots, n\} \) and that the graph with Laplacian \( L_3 \) has PST from \( p \) to \( q \). Then for each \( \ell = 1, \ldots, n \), \( w_1 \lambda^{(1)}_{\ell} + w_2 \lambda^{(2)}_{\ell} \equiv (1 - h_{p\ell} h_{q\ell}) \mod 4 \) and \( w_1 \lambda^{(1)}_{\ell} - w_2 \lambda^{(2)}_{\ell} + 2w_2 d_2 \equiv (1 - h_{p\ell} h_{q\ell}) \mod 4 \). In particular, \( 2w_2 d_2 \equiv 0 \mod 4 \), i.e., \( w_2 d_2 \) is even. Note that if \( w_1 \) and \( w_2 \) are both even, then \( h_{p\ell} h_{q\ell} = 1 \) for \( \ell = 1, \ldots, n \), which is impossible.
If \( w_1 \) is odd and \( w_2 \) is even, then \( w_1 \lambda^{(1)}_{\ell} + w_2 \lambda^{(2)}_{\ell} \equiv \lambda^{(1)}_{\ell} \mod 4 \), so that \( \lambda^{(1)}_{\ell} \equiv (1 - h_{p\ell} h_{q\ell}) \mod 4, \ell = 1, \ldots, n \). Hence \( G_1 \) has PST from \( p \) to
q. Similarly, if \( w_1 \) is even and \( w_2 \) is odd, then necessarily \( d_2 \) is even, and as above \( G_2 \) has PST from \( p \) to \( q \).

If \( w_1 \) and \( w_2 \) are both odd, then necessarily \( d_2 \) is even. Also \( w_1 \lambda_\ell^{(1)} + w_2 \lambda_\ell^{(2)} \equiv \lambda_\ell^{(1)} + \lambda_\ell^{(2)} \equiv (1 - h_{pd}h_{qd}) \mod 4, \ell = 1, \ldots, n \). We deduce that the graph with Laplacian \( L_1 + L_2 \) has PST from \( p \) to \( q \).

2. If \( p, q \in \{n + 1, \ldots, 2n\} \) and the graph with Laplacian \( L_3 \) has PST from \( p \) to \( q \), the conclusions (a), (b), and (c) follow analogously to Case 1 above.

3. Suppose that \( p \in \{1, \ldots, n\} \), \( q \in \{n + 1, \ldots, 2n\} \) and that the graph with Laplacian \( L_3 \) has PST from \( p \) to \( q \). Set \( \hat{q} = q - n \). Then for each \( \ell = 1, \ldots, n \), we have

\[
\begin{align*}
w_1 \lambda_\ell^{(1)} + w_2 \lambda_\ell^{(2)} &\equiv (1 - h_{pd}h_{q\hat{d}}) \mod 4, \quad (2) \\
w_1 \lambda_\ell^{(1)} - w_2 \lambda_\ell^{(2)} + 2w_2d_2 &\equiv (1 + h_{pd}h_{q\hat{d}}) \mod 4. \quad (3)
\end{align*}
\]

Summing equations (2) and (3), we find that \( 2w_1\lambda_\ell^{(1)} + 2w_2d_2 \equiv 2 \mod 4 \) and hence \( 2w_2d_2 \equiv 2 \mod 4 \) since all the eigenvalues of \( L_1 \) are even integers, and therefore \( w_2d_2 \) must be odd, i.e., \( w_2 \) is odd and \( d_2 \) is odd. We have the following two cases.

If \( w_1 \) is even, then (2) simplifies to \( \lambda_\ell^{(2)} \equiv (1 - h_{pd}h_{q\hat{d}}) \mod 4, \ell = 1, \ldots, n \), so for even \( w_1 \), and odd \( w_2 \) and \( d_2 \), \( G_2 \) has PST from \( p \) to \( \hat{q} \).

If \( w_1 \) is odd, then (2) simplifies to \( \lambda_\ell^{(1)} + \lambda_\ell^{(2)} \equiv (1 - h_{pd}h_{q\hat{d}}) \mod 4, \ell = 1, \ldots, n \), which shows that the integer-weighted graph with Laplacian \( L_1 + L_2 \) has PST from \( p \) to \( \hat{q} \).

The converses are straightforward. \( \Box \)

Note that when both \( w_1 \) and \( w_2 \) are even, the graph \( G_{1 \cup w_1 \cap w_2} G_2 \) does not have PST at time \( \pi/2 \). However, it might have PST at some other time. To see this, we decompose the two integer weights \( w_j \) as \( w_j = 2^r b_j \) (for \( j = 1, 2 \)), where \( b_j \) are odd integers. Let \( r = \min(r_1, r_2) \). Then the PST property of the graph with Laplacian \( \frac{1}{2} L_3 \) at time \( \pi/2 \) can be determined according to Theorem 4. In the case that PST occurs, the graph \( G_{1 \cup w_1 \cap w_2} G_2 \) would then have PST at time \( \pi/2^{r+1} \). Also note that Theorem 4 is true for any graphs whose Laplacian eigenvalues are all even integers (including non integer-weighted graphs).

**Remark 2.** Assume that \( G_1 \) and \( G_2 \) are two graphs on \( 2^m \) vertices for \( m \geq 2 \) and that they are diagonalizable by the same Hadamard matrix. Suppose that \( G_1 \) has PST from vertex \( p \) to vertex \( q \), and \( G_2 \) has all its eigenvalues being multiples
of 4 and that its degree \( d_2 \) is odd (for example, a disjoint union of \( 2^{m-r} \) copies of \( K_{2^r} \) for \( 2 \leq r \leq m \)). Then \( G_1 \odot G_2 \) has PST from \( p \) to \( q + 2^m \) according to Case 3(b) in Theorem 4. Similarly, \( G_2 \odot G_1 \) has PST from vertex \( p \) to \( q \) if \( d_1 \) is even (Case 1(c)), and it has PST from vertex \( p \) to \( q + 2^m \) if \( d_1 \) is odd (Case 3(b)).

The requirement that both graphs are diagonalizable by the same Hadamard matrix is necessary for Theorem 4 to hold. As a concrete example, let \( G_1 \) be equal to \( K_8 \) with a \( K_3 \) removed, \( G_2 \) be equal to the 3-cube, \( w_1 = 2 \) and \( w_2 = 1 \) (and \( d_2 = 3 \)). Then \( G_1 \odot_{w_2} G_2 \) is equal to

\[
\begin{bmatrix}
13 & 0 & 0 & -2 & -2 & -2 & -2 & 0 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\
0 & 13 & 0 & -2 & -2 & -2 & -2 & -1 & 0 & 0 & -1 & 0 & 0 & 0 \\
0 & 0 & 13 & -2 & -2 & -2 & -2 & -1 & 0 & 0 & -1 & 0 & -1 & 0 \\
-2 & -2 & -2 & 17 & -2 & -2 & -2 & -2 & 0 & -1 & -1 & 0 & 0 & -1 \\
-2 & -2 & -2 & -2 & 17 & -2 & -2 & -2 & 0 & -1 & 0 & -1 & 0 & -1 \\
-2 & -2 & -2 & -2 & -2 & 17 & -2 & -2 & 0 & 0 & 0 & 0 & 0 & -1 \\
-2 & -2 & -2 & -2 & -2 & -2 & 17 & 0 & 0 & 0 & 0 & -1 & 0 & -1 \\
0 & -1 & -1 & 0 & 0 & 13 & 0 & 0 & -2 & -2 & -2 & -2 & 2 & -2 \\
-1 & 0 & 0 & -1 & 0 & 0 & 13 & 0 & -2 & -2 & -2 & -2 & 2 & -2 \\
-1 & 0 & 0 & -1 & 0 & 0 & 13 & 0 & -2 & -2 & -2 & -2 & 2 & -2 \\
0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & -1 & -2 & -2 & -2 & -2 & -2 \\
-1 & 0 & 0 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & -1 & 0 & 0 & -1 & 0 & 0 & -1 & -2 & -2 & -2 & -2 & -2 & -2 \\
0 & 0 & -1 & 0 & 0 & 0 & -1 & -2 & -2 & -2 & -2 & -2 & -2 & 17 \\
0 & 0 & 0 & -1 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & -2 \\
0 & 0 & 0 & -1 & 0 & 0 & -1 & -1 & 0 & 0 & 0 & 0 & 0 & -2 \\
0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0
\end{bmatrix}
\]

There is no PST at time \( \pi/2 \), though the parameters are set up so that they satisfy 3(a) of Theorem 4 (but not the hypothesis of both Laplacians being diagonalized by the same Hadamard). Thus, unlike a similar result \[14, \text{Theorem 5.2}\] for the “\( \kappa \)” operation (which uses the adjacency matrices), graphs whose Laplacian matrices aren’t diagonalizable by the same Hadamard matrix do not necessarily satisfy the conclusion of the theorem. This may be due to the difference between Laplacian dynamics and adjacency dynamics.

The following corollary to Theorem 4 provides an instance where the statement of the theorem simplifies considerably, and generalizes the known fact that the unweighted hypercube graph has PST.

**Corollary 2.** Suppose \( w_1, w_2, \ldots, w_n \) are nonzero integers, exactly \( d \) of which are odd, and consider the weighted hypercube \( C_n := (w_1 K_2) \square (w_2 K_2) \square \cdots \square (w_n K_2) \).
For each vertex $u$ of $C_n$, there is a vertex $v$ at distance $d$ from $u$ such that there is perfect state transfer in $C_n$ from $u$ to $v$ at time $t_0 = \pi/2$.

**Proof.** We prove the result by induction on $n$. For the base case, we simply note that it is straightforward to verify that the weighted 1-cube $w_1 K_2$ has perfect state transfer at time $t = \pi/2$ if and only if $w_1$ is an odd integer.

For the inductive hypothesis, we use Theorem 4 with $G_1 = C_n$ (which we will assume has perfect state transfer at time $t = \pi/2$ from vertex $j$ to $k$, which are a distance of $d$ apart) and $G_2$ is the graph on the same number of vertices where every vertex has a self-loop (of weight 1) and no other edges (note that this graph has perfect state transfer between any vertex and itself at any time). Then it is straightforward to verify that the graph $G_1 \odot w_{n+1} G_2$ is exactly the weighted $(n + 1)$-cube:

$$G_1 \odot w_{n+1} G_2 = (w_{n+1} K_2) \square C_n = (w_{n+1} K_2) \square (w_1 K_2) \square (w_2 K_2) \square \cdots \square (w_n K_2).$$

So condition 1(a) of Theorem 4 tells us that if $w_{n+1}$ is even then $G_1 \odot w_{n+1} G_2$ has perfect state transfer at time $t_0 = \pi/2$ from vertex $j$ to $k$ (which still have a distance of $d$ from each other). On the other hand, if $w_{n+1}$ is odd then condition 3(b) of Theorem 4 says that $G_1 \odot w_{n+1} G_2$ has perfect state transfer at time $t = \pi/2$ from vertex $j$ to $k + 2^n$ (which have a distance of $d + 1$ from each other). By noting that the particular labelling of the weights is irrelevant (i.e., permute the indices of the weights so that $G_1 \odot w_{n+1} G_2 = (w_1 K_2) \square (w_2 K_2) \square \cdots \square (w_{n+1} K_2) = C_{n+1})$, this completes the inductive step and the proof.

**Example 1.** From Lemma 9 and Proposition 10 of [5], one can conclude that there is no unweighted graph of order 12 that is Hadamard diagonalizable and exhibits PST. However, it is easy to construct weighted graphs of this type. Let $G_1$

16
be the graph whose Laplacian is

\[
L_1 = \frac{1}{3} \begin{bmatrix}
18 & 0 & -1 & -1 & -1 & -3 & -3 & -3 & -3 & -1 & -1 & -1 \\
0 & 18 & -1 & -1 & -1 & -3 & -3 & -3 & -1 & -3 & -1 & -1 \\
-1 & -1 & 18 & -2 & -2 & 0 & -2 & 0 & -2 & -2 & -4 & -2 \\
-1 & -1 & -2 & 18 & -4 & 0 & 0 & -2 & -2 & -2 & -2 & -2 \\
-1 & -1 & -2 & -4 & 18 & -2 & -2 & 0 & -2 & 0 & -2 & -2 \\
-3 & -3 & 0 & 0 & -2 & 18 & -2 & -2 & 0 & -2 & -2 & -2 \\
-3 & -3 & -2 & 0 & -2 & -2 & 18 & -2 & -2 & 0 & 0 & 0 \\
-3 & -3 & -2 & -2 & 0 & -2 & -2 & 18 & 0 & -2 & -4 & -4 \\
-3 & -3 & -2 & -2 & 0 & -2 & -2 & 0 & 18 & 0 & -2 & -2 \\
-1 & -1 & -4 & -2 & -2 & -2 & 0 & -2 & -2 & 0 & 18 & -2 \\
-1 & -1 & -2 & -2 & -2 & 0 & 0 & -4 & -2 & -2 & 18 & -2 \\
\end{bmatrix}
\]

Then one can easily verify that \( L_1 \) is Hadamard diagonalizable by the order 12 Hadamard

\[
H = \begin{bmatrix}
1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\
1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1 & 1 & -1 \\
1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & -1 & 1 & 1 \\
1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 \\
1 & -1 & 1 & 1 & -1 & -1 & -1 & -1 & -1 & -1 & 1 & 1 \\
1 & 1 & -1 & 1 & 1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\
1 & 1 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\
\end{bmatrix}
\]

and that the \((1, 2)\) entry of \( e^{i\pi/2}L_1 \) is 1, thus showing that \( L_1 \) exhibits PST between vertices 1 and 2 at time \( t_0 = \pi/2 \). Let \( G_2 = K_{12} \), which we note is Hadamard diagonalizable by \( H \) but does not exhibit PST, and let \( w_1 = 5 \) and \( w_2 = 2 \). Direct computation shows that all the eigenvalues of \( L_1 \) are even integers. Hence Theorem [4] still applies here, and Case 1(a) of the theorem tells us that \( G_1 \circ \circ_2 \circ G_2 \) has PST from vertex 1 to vertex 2 at time \( t_0 = \pi/2 \). One can indeed verify that
\[ L_3 = \begin{bmatrix} 5L_1 + 2D_2 & -2A_2 \\ -2A_2 & 5L_1 + 2D_2 \end{bmatrix}, \] where \( D_2 = 11I \) and \( A_2 = J - I \) (where \( J \) is the all-ones matrix), is Hadamard diagonalizable by \( \begin{bmatrix} H & H \\ H & -H \end{bmatrix} \) with eigenvalues (in the order determined by that diagonalization) equal to 0, 54, 64, 64, 64, 64, 54, 54, 44, 54, 44, 50, 60, 60, 60, 60, 60, 50, 50, 50, and 50. Furthermore, by checking the \((1, 2)\) entry of \( e^{i(\pi/2)L_3} \) we see that this graph exhibits PST between vertices 1 and 2 at time \( t_0 = \pi/2 \).

**Remark 3.** For each \( k \geq 3 \) and each \( d \) with \( k + 1 \leq d \leq 2^k - 2 \), we can construct a graph that is \( d \)-regular, unweighted, connected, and non-bipartite on \( 2^k \) vertices, that is diagonalizable by the standard Hadamard matrix and has PST at time \( t_0 = \pi/2 \). This can be done with cubelike graphs by using Theorem 1. To ensure the cubelike graph is connected, we just need to make sure the connection set contains a basis of \( \mathbb{Z}_2^k \) when considered as a vector space. Let us take the standard ordered basis: \( e_1, \ldots, e_k \). Assume they form the set \( T \). For \( d = k + 1 \), take the connection set \( C = T \cup \{e_1 + e_2\} \). Then the induced subgraph on vertices \( 0, e_1, e_2, e_1 + e_2 \) is \( K_4 \); hence the corresponding cubelike graph is not bipartite. Also note that the sum of the elements in \( C \) is not 0 for \( k \geq 3 \). For \( d > k + 1 \), we always keep \( C \) as a subset of the connection set \( S \) (\( |S| = d, 0 \notin S \)). If the sum of all elements in \( S \) is not 0, then the cubelike graph \( G(S) \) is a desired graph. On the other hand, if the sum of all elements in \( S \) is 0, then we delete some element \( c_0 \) from the set \( S \setminus C \). Denote the set \( S \setminus \{c_0\} \) by \( S_0 \) and we know the sum of all its elements is \( c_0 \neq 0 \) (in \( \mathbb{Z}_2^k \), every element has itself as its inverse). Finally, we pick any element \( c_1 \in \mathbb{Z}_2^k \setminus (S \cup \{0\}) \) (this set has cardinality \( 2^k - d - 1 > 0 \)) and form a new set \( S_1 = S_0 \cup \{c_1\} \). Then \( S_1 \) has cardinality \( d \) and the sum of all its element is \( c = c_0 + c_1 \neq 0 \). Hence there is PST from \( u \) to \( u + c \) at time \( \pi/2 \) in the connected (since \( S_1 \) is a generating set of the group \( \mathbb{Z}_2^k \)) nonbipartite cubelike graph \( G(S_1) \).

This remark can be stated as follows. As a means of highlighting the utility of the merge operation, we present an alternate proof that constructs such graphs using the merge.

**Theorem 5.** Suppose that \( k \in \mathbb{N} \) with \( k \geq 3 \). For each \( d \in \mathbb{N} \) with \( k + 1 \leq d \leq 2^k - 2 \), there is a connected, unweighted, non-bipartite graph that is

1. diagonalizable by the standard Hadamard matrix of order \( 2^k \),
2. \( d \)-regular, and
Proof. For every integer $k \geq 3$, it is easy to see that the complement of a perfect matching (disjoint union of $2^{k-1}$ copies of $K_2$) is a $(2^k - 2)$-regular graph with the desired properties. So we just need to prove the result for $k + 1 \leq d \leq 2^k - 3$. We proceed by induction on $k$. For $k = 3$, it is straightforward to check that $(K_{2,2} \Box K_2)^c$, $(K_{2,2} + K_{2,2})^c$ and $(K_2 + K_2 + K_2 + K_2)^c$ are $4$-, $5$-, and $6$-regular graphs, respectively, having the described properties. Now suppose the result holds for some fixed $k \geq 3$; that is, for each $d$ with $k + 1 \leq d \leq 2^k - 2$, we have a $d$-regular graph $G_{k,d}$ on $2^k$ vertices with the desired properties. To construct desired graphs on $2^{k+1}$ vertices, we split into two cases depending on the regularity $d$ of the graph that we are trying to construct.

Case 1: $(k + 1) + 1 \leq d \leq 2^k - 1$. Let the Laplacian matrix for $G_{k,d-1}$ be $L_{k,d-1}$. Consider the graph $K_2 \Box G_{k,d-1}$, This graph has $2^k + 1$ vertices and Laplacian $\begin{bmatrix} L_{k,d-1} + I & -I \\ -I & L_{k,d-1} + I \end{bmatrix}$. It is straightforward to see that this graph is $d$-regular, connected, non-bipartite (since $G_{k,d-1}$ is) and satisfies (1) and (3).

Case 2: $k + 4 \leq d \leq 2^{k+1} - 3$. For each $2 \leq r \leq k$, let $G_r$ be the disjoint union of $2^k - r$ copies of $K_{2r}$ and let $L_r$ denote its Laplacian matrix. Note that each eigenvalue of $L_r$ is congruent to 0 (mod 4); further, with a natural labelling of the vertices, $L_r$ is diagonalizable by the standard Hadamard matrix of order $2^k$.

Fix $d'$ with $k + 1 \leq d' \leq 2^k - 2$ and let $A_{k,d'}$ be the adjacency matrix of $G_{k,d'}$. Let $G^{(r)}_{k,d'} = G_r \circ G_{k,d'}$ be the graph on $2^{k+1}$ vertices whose Laplacian matrix is $L^{(r)}_{k,d'} = \begin{bmatrix} L_r + d'I & -A_{k,d'} \\ -A_{k,d'} & L_r + d'I \end{bmatrix}$. Then $G^{(r)}_{k,d'}$ is not bipartite (it has $K_4$ as an induced subgraph), and it is Hadamard diagonalizable by the standard Hadamard matrix. By Remark it also has PST between a pair of distinct vertices. It is regular of degree $d' + 2r - 1$. Also in the notation of Theorem $-\Lambda_2 + 2d'I$ has positive diagonal entries (since $G_{k,d'}$ is not bipartite) and so we deduce that the nullity of $L^{(r)}_{k,d'}$ is 1 and that $G^{(r)}_{k,d'}$ is connected. Thus $G^{(r)}_{k,d'}$ is a graph on $2^{k+1}$ vertices, satisfying the desired properties. We denote it as $G_{k+1,d'+2r-1}$.
Thus we have produced the desired graphs whose degrees fall in the set

\[ [k + 2, 2^k - 1] \cup \bigcup_{r=2}^{k} [k + 2^r, 2^k + 2^r - 3]. \]  

For \( k = 3 \), this set covers the integers 5, 6, 7, 8, 9, 11, 12, 13. From Proposition 1 we know that if \( G = (K_{2,2} + K_{2,2})^c \), our 5-regular graph on 8 vertices satisfying the desired properties, then the graph \( G^c \lor G^c \) of order 16 is 10-regular and has the desired properties. So the result is also true for graphs on 2^4 vertices.

For \( k \geq 4 \) we have \( k + 4 \leq 2^{k-1} \). Then for any \( r \leq k - 1 \), we have \( k + 4 + 2^{r+1} \leq 2^{k-1} + 2^{r+1} = 2^{k-1} + 2^r + 2^r \leq 2^{k-1} + 2^{k-1} + 2^r = 2^k + 2^r \), which in turn implies that \( k + 2^{r+1} \leq 2^k + 2^r - 3 \). It follows that the set (4) contains all of the integers in \( [k + 2, 2^k + 2^r - 3] \).

**Remark 4.** Note that for \( 2^{k+1} + 1 \leq d \leq 2^{k+1} - 2 \), we can also construct a \( d \)-regular graph with the desired properties on \( 2^{k+1} \) vertices using the join operation. From the induction hypothesis, we have a graph \( G_{k,d} \) with the desired properties for \( k + 1 \leq d \leq 2^k - 2 \). Now we use the result in Proposition 1: if \( G \) is a Hadamard diagonalizable graph on \( n \geq 4 \) vertices and that \( G \) has PST at time \( \pi/2 \), then its complement also has PST at the same time, then we get a non-empty \( d \)-regular Hadamard diagonalizable PST graph \( G \) for each \( d \) such that \( 1 \leq d \leq 2^k - 2 \). Then the graph \( G \lor G \) has PST at time \( t_0 = \pi/2 \) and is diagonalizable by the standard Hadamard matrix, whose regularity is \( 2^k + d \), ranging from \( 2^k + 1 \) to \( 2^k + 2^k - 2 \). Since \( G \) is not empty, \( G \lor G \) has cycles of length 3, and therefore it is not bipartite.

### 5. PST for graphs with non-integer weights

We now consider some ways in which our results generalize to the case of Hadamard diagonalizable graphs with non-integer edge weights. In the case where all of the edge weights are rational, the idea is rather straightforward.

**Proposition 2.** Suppose the graph \( G_1 \) with Laplacian \( L_1 \) is a rational-weighted Hadamard diagonalizable graph, and let \( \text{lcm} \) be the least common multiple of the denominators of its edge weights, and \( \text{gcd} \) be the greatest common divisor of all the new integer edge weights \( \text{lcm} \cdot w(j,k) \). Then \( G_1 \) has PST at time \( t_1 = \frac{\text{lcm}}{\text{gcd}} \cdot \pi/2 \) if and only if the integer-weighted Hadamard diagonalizable graph \( G_2 \) with Laplacian \( L_2 = \frac{\text{lcm}}{\text{gcd}} L_1 \) has PST at time \( t_0 = \pi/2 \) between the same pair of vertices.
Proof. The result follows simply from noticing that for each \( j \) and \( k \) we have
\[
|e_j^T e^{it_0L_2} e_k|^2 = |e_j^T e^{it_0\frac{\ln q}{\ln p} L_1} e_k|^2 = |e_j^T e^{it_1 L_1} e_k|^2, \tag{5}
\]
and \( G_1 \) has PST between vertex \( j \) and vertex \( k \) at time \( t_1 \) if and only the rightmost quantity in (5) equals 1, while \( G_2 \) has PST at time \( t_0 \) if and only if the leftmost quantity in (5) equals 1.

While we are not able to extend Proposition 2 to the case of irrational weights directly—in general such a graph may not exhibit PST at any time—it is true at least that the resulting graph has pretty good state transfer when exactly one of the two weights in \( G_1 \circ w_1 \circ w_2 \ G_2 \) is irrational. Before giving the theorem, we recall the following result about approximating an irrational real number with rational numbers.

**Theorem 6 ([22]).** Let \( o \) denote the odd integers and \( e \) denote the even integers. Then for every real irrational number \( w \), there are infinitely many relatively prime numbers \( u, v \) with \( [u, v] \) in each of the three classes \([o, e], [e, o], \text{and } [o, o] \), such that the inequality \( |w - u/v| < 1/v^2 \) holds.

For the graph \( G_1 \circ w_1 \circ w_2 \ G_2 \), we say it has parameters \([w_1, w_2, d_2]\), where as in Theorem 4, \( d_2 \) denotes the degree of \( G_2 \). In particular, if \( w_1, w_2, \text{and } d_2 \) are all odd integers, we say the graph \( G_1 \circ w_1 \circ w_2 \ G_2 \) has type \([o, o, o]\). We will denote the set of irrational numbers by \( \overline{\mathbb{Q}} \).

**Theorem 7.** Assume that \( G_1 \) and \( G_2 \) are integer-weighted graphs on \( n \) vertices, both of which are diagonalizable by the same Hadamard matrix \( H \). Let \( d_2 \) be the degree of \( G_2 \). Let \( L_1 \) and \( L_2 \) denote the Laplacian matrices of \( G_1 \) and \( G_2 \), respectively. Suppose that one of \( w_1, w_2 \) is rational and the other is irrational, and suppose that \( p, q \in \{1, \ldots, n\} \). Then the weighted graph \( G_1 \circ w_1 \circ w_2 \ G_2 \) has PGST as stated in the following cases.

1. Suppose that \( G_1 \) has PST from \( p \) to \( q \) at time \( \pi/2 \). Then \( G_1 \circ w_1 \circ w_2 \ G_2 \) has PGST from \( p \) to \( q \) and from \( p + n \) to \( q + n \).
2. Suppose that \( G_2 \) has PST from \( p \) to \( q \) at time \( \pi/2 \). If \( d_2 \) is even, then \( G_1 \circ w_1 \circ w_2 \ G_2 \) has PGST from \( p \) to \( q \) and from \( p + n \) to \( q + n \). If \( d_2 \) is odd, then \( G_1 \circ w_1 \circ w_2 \ G_2 \) has PGST from \( p \) to \( q + n \) and from \( q \) to \( p + n \).
3. Suppose that the graph with Laplacian \( L_1 + L_2 \) has PST from \( p \) to \( q \) at time \( \pi/2 \). If \( d_2 \) is even, then \( G_1 \circ w_1 \circ w_2 \ G_2 \) has PGST from \( p \) to \( q \) and from \( p + n \) to \( q + n \). If \( d_2 \) is odd, then \( G_1 \circ w_1 \circ w_2 \ G_2 \) has PGST from \( p \) to \( q + n \) and from \( q \) to \( p + n \).
Before proving this result, we note that it can alternatively be proved via Kronecker’s theorem using the techniques of [4]. However, this would require proving that vertices $p$ and $q$ are strongly cospectral, as well as some knowledge of eigenvalues and eigenprojection matrices, so we instead give the following proof that is somewhat more self-contained.

**Proof.** As in the proof of Theorem 4 Without loss of generality we assume that $H$ is a normalized Hadamard matrix. Assume $w_1$ is rational and $w_2$ is irrational (case 1). We denote the graph $G_1 \circ w_1 \circ G_2$ as $G_3$, with corresponding Laplacian $L_3$. It suffices to consider $w_1$ odd. Indeed, if $w_1 = \frac{a}{b}$, with $a$ and $b$ being relatively prime integers, assume $a = 2^r k$ where $r \in \mathbb{N}$ and $k$ odd, then $e^{it L_3} = e^{it \frac{a}{b}(L_3 b/2^r)}$ so that $L_3 b/2^r$ is the Laplacian of the graph $G_1 \circ w_1 \circ G_2$ where $k$ is odd and $w_3 b/2^r$ is irrational. Note that if $L_3 b/2^r$ has PGST, then so does $L_3$. Thus, for notational simplicity, we consider $w_1$ odd.

We approach $w_2$ with fractions $u/v$ such that $|w_2 - u/v| < 1/v^2$. For each such pair of $u, v$, we denote the graph $G_1 \circ u \circ G_2$ as $G_4$, and the graph $G_1 \circ w_2 \circ G_2$ as $G_5$. In particular, the Laplacian of $G_3$ is the sum of the Laplacian of $G_4$ with the Laplacian of $G_5$. Denote the Laplacian matrices of $G_4$ and $G_5$ as $L_4$ and $L_5$, respectively. Now consider the integer-weighted graph $G'_4 = G_1 \circ w_1 \circ u \circ G_2$, then its Laplacian is $vL_4$ and has parameters $[w_1, u, d_2]$.

There are now a number of cases to consider. If $[u, v]$ is of type $[o, e]$ and $d_2$ is even, the graph $G'_4$ is of type $[e, o, e]$. From Theorem 4 we know, if $G_2$ has PST from $p$ to $q$ at $\pi/2$, then $G'_2$ has PST at $\pi/2$ from $p$ to $q$ and from $p + n$ to $q + n$ (Case 1(b), 2(b)). If $[u, v]$ is of type $[o, e]$ and $d_2$ is odd, the graph $G'_4$ is of type $[e, o, o]$. From Theorem 4 we know that if $G_2$ has PST at $\pi/2$ from $p$ to $q$ at $\pi/2$, then $G'_4$ has PST at $\pi/2$ from $p$ to $q + n$ and from $q$ to $p + n$ (Case 3(a)).

If $[u, v]$ is of type $[e, o]$, then the graph $G'_4$ is of type $[o, e, f]$, where $f$ denotes the parity of $d_2$. From Theorem 4 we know that if $G_1$ has PST from $p$ to $q$ at $\pi/2$, then $G'_4$ has PST at $\pi/2$ from $p$ to $q$ and from $p + n$ to $q + n$ (Case 1(a), 2(a)).

If $[u, v]$ is of type $[o, o]$ and $d_2$ is even, the graph $G'_4$ is of type $[o, e, o]$. From Theorem 4 we know that if the graph with Laplacian $L_1 + L_2$ has PST from $p$ to $q$ at $\pi/2$, then $G'_4$ has PST from $p$ to $q$ and from $p + n$ to $q + n$ (Case 1(c), 2(c)). If $[u, v]$ is of type $[o, o]$ and $d_2$ is odd, the graph $G'_4$ is of type $[o, o, o]$. From Theorem 4 we know that if the integer weighted graph with Laplacian $L_1 + L_2$ has PST from $p$ to $q$ at $\pi/2$, then $G'_4$ has PST from $p$ to $q + n$ and from $q$ to $p + n$ (Case 3(b)).

Similarly we can get the results when $w_1$ is irrational and $w_2$ is rational (case 2). (We can assume $w_2$ is odd by way of a similar argument to $w_1$ being odd in
case 1.)

For all the above cases, \( G_4 \) has PST at time \( t_0 = v\pi/2 \). Next, we recall the following result from [16, Theorem 4] (here we take the absorbed constant factor \( t_0 \) out): Suppose PST occurs for the graph with Laplacian matrix \( L \) and assume that \( \hat{L} = t_0(L + L_0) \) due to a small nonzero edge-weight perturbation \( L_0 \). Then

\[
1 - |e_j^T e^{it_0(L + L_0)} e_k|^2 \leq 2\|t_0L_0\| + \|t_0L_0\|^2 - \|t_0L_0\|^3. \tag{6}
\]

Now, \( G_4 \) is a graph with PST at time \( t_0 \), and \( L_3 = L_4 + L_5 \). Then the fidelity of state transfer of \( G_3 \) between the corresponding pair of vertices satisfies

\[
|e_j^T e^{it_0L_3} e_k|^2 \geq 1 - 2\|t_0L_5\| - \|t_0L_5\|^2 + \|t_0L_5\|^3
\geq 1 - 2cn\pi/(2v) - (cn\pi/(2v))^2 + (cn\pi/(2v))^3,
\]

where \( c \) is the maximum edge weight in \( G_2 \). Since there are infinitely such integers \( v \), the expression on the right hand side in the above inequality can be made as close to one as possible.

It is known (see [18]) that if there is perfect state transfer from vertex \( j \) to vertex \( k \) at time \( t_0 \), and perfect state transfer from vertex \( j \) to vertex \( l \) at time \( t_1 \), then necessarily \( k = l \). The following example, which is a straightforward consequence of Theorem [7] shows that the situation with respect to pretty good state transfer is markedly different. This is a potentially important application to routing—the task of choosing between several possible recipients of the state.

**Example 2.** Consider the unweighted graphs \( G_1, G_2 \) with the following Laplacian matrices:

\[
L_1 = \begin{bmatrix}
3 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\
-1 & 3 & 0 & -1 & 0 & -1 & 0 & 0 \\
-1 & 0 & 3 & -1 & 0 & 0 & -1 & 0 \\
0 & -1 & -1 & 3 & 0 & 0 & 0 & -1 \\
-1 & 0 & 0 & 3 & -1 & -1 & 0 & 0 \\
0 & -1 & 0 & 0 & -1 & 3 & 0 & -1 \\
0 & 0 & -1 & 0 & -1 & 0 & 3 & -1 \\
0 & 0 & 0 & -1 & 0 & -1 & -1 & 3
\end{bmatrix}
\]
which has PST at time $\pi/2$ for the pairs (1, 8), (2, 7), (3, 6), (4, 5), and

$$L_2 = \begin{bmatrix}
3 & 0 & -1 & -1 & -1 & 0 & 0 & 0 \\
0 & 3 & -1 & -1 & 0 & -1 & 0 & 0 \\
-1 & -1 & 3 & 0 & 0 & 0 & -1 & 0 \\
-1 & -1 & 0 & 3 & 0 & 0 & 0 & -1 \\
-1 & 0 & 0 & 0 & 3 & 0 & -1 & -1 \\
0 & -1 & 0 & 0 & 0 & 3 & -1 & -1 \\
0 & 0 & -1 & 0 & -1 & -1 & 3 & 0 \\
0 & 0 & 0 & -1 & -1 & -1 & 0 & 3 \\
\end{bmatrix}$$

which has PST at time $\pi/2$ for the pairs (1, 6), (2, 5), (3, 8), (4, 7). It turns out that $L_1 + L_2$ has PST at time $\pi/2$ between the pairs (1, 3), (2, 4), (5, 7), (6, 8). From the above collection of cases, we find for example that if $w_1 \in Q$ and $w_2 \in \overline{Q}$ (or $w_1 \in \overline{Q}$ and $w_2 \in Q$), then $G_1 \circ \circ \circ G_2$ has the intriguing property that there is PGST between the pairs (1, 8), (1, 11), (1, 14) (among others).

6. Optimality

6.1. Timing errors

In [16], the authors analyse the sensitivity of the probability of state transfer in the presence of small perturbations. Bounds on the probability of state transfer with respect to timing errors and with respect to manufacturing errors were given in the most general setting where no information is known about the graph in question. Specifically, suppose that under XXX dynamics, a graph $G$ on $n$ vertices has PST from vertex 1 to vertex 2 at time $t_0$. Suppose further that there is a small perturbation so that the readout time is instead $t_0 + h$, where $|h| < \frac{\pi}{\lambda_n}$, and where $\lambda_n$ is the largest eigenvalue of the corresponding Laplacian. Decompose the Laplacian as $L = Q\Lambda Q^T$, where $\Lambda = \text{diag}(\lambda_1 = 0, \lambda_2, \ldots, \lambda_n)$, with $0 < \lambda_2 \leq \cdots \leq \lambda_n$, and $Q$ is an orthogonal matrix of corresponding eigenvectors. If $q_1$ and $q_2$ are the first and second columns of $Q^T$, respectively, then for some $\theta \in \mathbb{R}$ we have $e^{i\theta}q_1 = e^{it_0\lambda_1}q_2$. Setting $M = \text{diag}(e^{ih\lambda_1}, \ldots, e^{ih\lambda_n})e^{i\theta}$, it follows that

$$p(t_0) - p(t_0 + h) = 1 - |q_1^TMq_1|^2.$$
In the special case that $G$ is Hadamard diagonalizable, we have $Q = \frac{1}{\sqrt{n}} H$, where $H$ is a Hadamard matrix, so we can say more. In that case, 

$$|q_1^T M q_1| = \frac{1}{n} \left| \sum_{j=1}^{n} e^{i \lambda_j} \right|. \quad (7)$$

This suggests that, in order to find a lower bound for $|q_1^T M q_1|$ (and thus an upper bound for $p(t_0) - p(t_0 + h)$), the goal should be to make the numbers $e^{i \lambda_j}$ as closely-spaced on the complex unit circle as possible. This agrees with the known fact that minimizing the spectral spread has the effect of maximizing the bound for the fidelity of state transfer due to timing errors [17]. Thus, this remark is not surprising but rather confirms the known rule while at the same time providing a more accurate bound on timing errors for Hadamard diagonalizable graphs.

### 6.2. Manufacturing errors: sparsity of graphs with PST

It is desirable to minimize the number of edges that need to be engineered in a graph (so as to minimize manufacturing errors), so one question of interest in the theory of perfect state transfer is how sparse a graph with perfect state transfer can be. Among the sparsest known graph with PST is the $k$-cube, which has $2^k$ vertices, each with degree $k$. We now show that if we restrict our attention to Hadamard diagonalizable unweighted graphs, then for $k \leq 4$ the $k$-cube is indeed the sparsest connected graph with PST.

**Theorem 8.** Let $G$ be a simple, connected, unweighted $r$-regular graph on $n$ vertices. Suppose further that $G$ is Hadamard diagonalizable, has perfect state transfer at $\pi/2$, and that $r \leq 4$. Then $n \leq 2^r$.

**Proof.** If $L$ is the Laplacian of $G$ then the result follows by computing some quantities of the form $\text{Tr}(L^k)$ ($k \geq 0$ is an integer) in two different ways. First, if $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of $L$ then $\text{Tr}(L^k) = \sum_{j=1}^{n} \lambda_j^k$, and we know by the Gershgorin circle theorem that $0 \leq \lambda_j \leq 2r$ for each $j$. On the other hand, $L = rI - A$, where $A$ is the adjacency matrix of $G$, so $\text{Tr}(L) = rn - \text{Tr}(A)$ and $\text{Tr}(L^2) = r^2n - 2r \text{Tr}(A) + \text{Tr}(A^2)$. Since $A$ is simple, we know that $\text{Tr}(A) = 0$ and it is straightforward to compute $\text{Tr}(A^2) = rn$. Thus we have the following system of equations:

$$\sum_{j=1}^{n} \lambda_j = rn \quad \text{and} \quad \sum_{j=1}^{n} \lambda_j^2 = rn(r+1).$$
If we let $c_\lambda$ denote the number of eigenvalues of $L$ equal to $\lambda$ (with the convention that if $\lambda$ is not an eigenvalue, then $c_\lambda = 0$), then these equations tell us that

$$\sum_{j=1}^r (2j)c_{2j} = rn \quad \text{and} \quad \sum_{j=1}^r (2j)^2 c_{2j} = rn(r + 1). \quad (8)$$

If we add in the equation $\sum_{j=1}^r c_{2j} = n - 1$ (since one of the eigenvalues equals 0), then we have a system of 3 linear equations in the variables $n, c_2, c_4, \ldots, c_{2r}$. If $r \leq 2$ then it is straightforward to solve this system of equations to get $n = 2^r$. If $r = 3$ then by adding the equation $c_2 + c_6 = c_4 + 1$ (since we know that half of $L$’s eigenvalues must belong to each equivalence class mod 4) we can similarly solve the system of equations to get $n = 8 = 2^3$.

For the $r = 4$ case, we use the Equations (8) together with the equation $c_2 + c_6 = c_4 + c_8 + 1$ (again, because the eigenvalues are split evenly between the mod 4 equivalence classes). These equations together can be reduced to the system of equations $c_2 = 3n/8 - 2$, $c_4 = 3n/8$, $c_6 = n/8 + 2$, and $c_8 = n/8 - 1$. To reduce this system further and get a unique solution, we need to compute $\text{Tr}(L^3)$ in two different ways (similar to at the start of the proof): $\text{Tr}(L^3) = \sum_{j=1}^n \lambda_j^3 = r^3 n - 3r^2 \text{Tr}(A) + 3r \text{Tr}(A^2) - \text{Tr}(A^3) = r^3 n + 3r^2 n - \text{Tr}(A^3)$. Since $\text{Tr}(A^3) \geq 0$ we arrive at the inequality $\sum_{j=1}^n \lambda_j^3 \leq r^2 n(r + 3)$, which is equivalent to $\sum_{j=1}^r (2j)^3 c_{2j} \leq r^2 n(r + 3)$. Plugging in $r = 4$ then gives

$$8c_2 + 64c_4 + 216c_6 + 512c_8 \leq 112n.$$ 

It is then straightforward to substitute the equations $c_2 = 3n/8 - 2$, $c_4 = 3n/8$, $c_6 = n/8 + 2$, and $c_8 = n/8 - 1$ into this inequality to get $n \leq 2^r = 16$, as desired. \(\square\)

It seems reasonable to believe that Theorem 8 could be generalized to arbitrary $r$, but the method of proof that we used does not seem to generalize in a straightforward way, as there are no more obvious equations or inequalities involving the $c_{2j}$’s that we can use. For example, if we try to extend the proof of Theorem 8 to the $r = 5$ case, we might try computing $\text{Tr}(L^4)$ in two different ways. However, we then end up with an equation involving both $-\text{Tr}(A^3)$ and $+\text{Tr}(A^4)$, and it is not clear how to bound such a quantity.
7. Acknowledgements

The authors are grateful to an anonymous referee, whose constructive comments resulted in improvements to the paper. N.J., S.K., and S.P. were supported by NSERC Discovery Grant number RGPIN-2016-04003, RGPIN/6123-2014, and 1174582, respectively; N.J. was also supported by a Mount Allison Marjorie Young Bell Faculty Fund; R.S. was supported through a NSERC Undergraduate Student Research Award; X.Z. was supported by the University of Manitoba’s Faculty of Science and Faculty of Graduate Studies.

References

[1] R. Alvir, S. Dever, B. Lovitz, J. Myer, C. Tamon, Y. Xu, H. Zhan, Perfect state transfer in Laplacian quantum walk, J. Algebraic Combin. 43 (2016), 801–826.

[2] R.J. Angeles-Canul, R.M. Norton, M.C. Opperman, C.C. Paribello, M.C. Russell, and C. Tamon, Quantum perfect state transfer on weighted join graphs, Int. J. Quantum Inf. 7 (2009), 1429–1445.

[3] R.J. Angeles-Canul, R.M. Norton, M.C. Opperman, C.C. Paribello, M.C. Russell, and C. Tamon, Perfect state transfer, integral circulants and join of graphs, Quant. Inform. Comput. 10 (2010), 325–342.

[4] L. Banchi, G. Coutinho, C. Godsil, and S. Severini, Pretty good state transfer in qubit chain–The Heisenberg Hamiltonian, J. Math. Phys. 58 (2017), 032202.

[5] S. Barik, S. Fallat, and S. Kirkland, On Hadamard diagonalizable graphs, Linear Algebra Appl. 435 (2011), 1885–1902.

[6] M. Bašić, Characterization of quantum circulant networks having perfect state transfer, Quantum Inf. Process. 12 (2013), 345–364.

[7] A. Bernasconi, C. Godsil, and S. Severini, Quantum networks on cubelike graphs, Phys. Rev. A 78 (2008), 052320.

[8] S. Bose, Quantum communication through an unmodulated spin chain, Phys. Rev. Lett., 91 (2003), 207901.
[9] J. Brown, C. Godsil, D. Mallory, A. Raz, and C. Tamon, *Perfect state transfer on signed graphs*, Quantum Inf. Comput. **13**, No. 5& 6 (2013), 0511–0530.

[10] C. K. Burrell and T. J. Osborne, *Bounds on the Speed of Information Propagation in Disordered Quantum Spin Chains*, Phys. Rev Lett. **99** (2007), 167201.

[11] W.-C. Cheung and C. Godsil, *Perfect state transfer in cubelike graphs*. Linear Algebra Appl. **435** (2011), 2468–2474.

[12] M. Christandl, N. Datta, T. C. Dorlas, A. Ekert, A. Kay, and A. J. Landahl, *Perfect transfer of arbitrary states in quantum spin networks*, Phys. Rev. A, **71** (2005), 032312.

[13] M. Christandl, N. Datta, A. Ekert, and A. J. Landahl, *Perfect State Transfer in Quantum Spin Networks*, Phys. Rev. Lett., **92** (2004), 187902.

[14] G. Coutinho and C. Godsil, *Perfect state transfer in products and covers of graphs*. Linear and Multilinear Algebra, **64** (2016), 235–246.

[15] G. De Chiara, D. Rossini, S. Montangero, and R. Fazio, *From perfect to fractal transmission in spin chains*, Phys. Rev. A **72** (2005), 012323.

[16] W. Gordon, S. Kirkland, C.-K. Li, S. Plosker, and X. Zhang, *Bounds on probability of state transfer with respect to readout time and edge weight*, Phys. Rev. A **93** (2016), 022309.

[17] A. Kay, *Perfect state transfer: beyond nearest-neighbor couplings*, Phys. Rev. A **73** (2006), 032306.

[18] A. Kay, *Basics of perfect communication through quantum networks*, Phys. Rev. A **84** (2011), 022337.

[19] A. Kay, *Quantum Error Correction for Noisy Quantum Wires*, arXiv:1507.06139 (2015).

[20] S. Kirkland, *Sensitivity analysis of perfect state transfer in quantum spin networks*, Linear Algebra Appl. **472** (2015), 1–30.

[21] R. Ronke, T. P. Spiller, and I. D’Amico, *Effect of perturbations on information transfer in spin chains*, Phys. Rev. A **83** (2011), 012325.
[22] W. T. Scott, *Approximation to real irrationals by certain classes of real fraction*, Duke J. Math., **12** (1940).

[23] A. Zwick, G. A. Álvarez, J. Stolze, and O. Osenda, *Robustness of spin-coupling distributions for perfect quantum state transfer*, Phys. Rev. A **84** (2011), 022311.