PERFECT QUANTUM STATE TRANSFER USING HADAMARD-DIAGONALIZABLE GRAPHS

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ABSTRACT. Quantum state transfer within a quantum computer 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 reverse-engineer graphs having perfect state transfer. We then introduce a new operation on graphs, which we call the *merge*, that takes two Hadamard-diagonalizable graphs on n vertices and produces a new graph on $2n$ vertices. We use this operation to produce 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.

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 [7] 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 identical to the input state of the sender at time $t = 0$.

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Many families of graphs have been found to exhibit PST, including the join of a weighted two-vertex graph with any regular graph [3], Hamming graphs [3] (see also [6, 10, 11]), a family of double-cone non-periodic graphs [2], and a family of integral circulant graphs [5] (see also [2]). It is easy to see that the cartesian product of two graphs having PST at the same time has PST [1, Sec. 3.3]. Much work has also been done with respect to analyzing the sensitivity [9, 12, 13, 15, 16, 17, 19], or even correcting errors [14], of quantum spin systems. Signed graphs and even graphs with arbitrary edge weights have also been considered (see [8] 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.

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 (which we focus on 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 $\mathbf{1}$ (the all-ones vector).

Our contribution to the theory of perfect state transfer is to detail a procedure for creating a graph with PST given two graphs on n vertices whose Laplacians are diagonalizable by the same Hadamard matrix and that satisfy certain conditions. This is accomplished through a new operation which we call the *merge* of the two graphs. This operation may be of interest in its own right, within the fields of graph theory and matrix analysis; here we simply use it as a tool to create new graphs exhibiting PST.

The constraint that the graphs must have 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 k-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 [4]; consequently the corresponding graph often exhibits PST between two of its vertices at time $t_0 = \pi/2$ (see Theorem 2 for a more specific statement).

In Section 2, we give a quick review of the graph theory and state transfer definitions that we will use. In Section 3, we give an eigenvalue characterization connecting a graph being Hadamard-diagonalizable and it having

PST between two of its vertices. In Section 4, we describe our "merge" 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. Typically $w(j,k)$ 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 ± 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 between every pair of vertices and *complete* if there is an edge between every pair of distinct vertices.

There are several different operations that can be performed to turn two graphs into a new (typically larger) graph. Specifically, given graphs $G = (V_1, E_1)$ and $H = (V_2, E_2)$, where V_1 and V_2 are disjoint sets of m and n vertices respectively, and E_1 and E_2 are the edges in the graph G and H respectively, then

(1) The *union* of G and H is the graph $G + H = (V_1 \cup V_2, E_1 \cup E_2)$;

(2) The *join* of G and H is the graph $G \vee H = (G^c + H^c)^c$: the graph on $m + n$ vertices where every vertex of G is connected to every vertex of H, and all of the original edges of G and H are retained as well; and
(3) The *Cartesian product* of G and H is the graph $G \square H = (V_1 \times V_2, E_3)$ where $V_1 \times V_2$ is the cartesian product of the two original sets of vertices, and there is an edge in $G \square H$ between vertices (g_1, h_1) and (g_2, h_2) if and only if either (i) $g_1 = g_2$ and there is an edge between h_1 and h_2 in H, or (ii) $h_1 = h_2$ and there is an edge between g_1 and g_2 in G.

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

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* [4]. Given a graph G on n vertices with corresponding Laplacian matrix L, if we can write $L = \frac{1}{n} H \Lambda H^T$ for some Hadamard H and diagonal matrix Λ, 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 [4, 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)* if $p(t_0) := |\mathbf{e}_j^T e^{it_0 \mathcal{H}} \mathbf{e}_k|^2 = 1$ 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 $e^{it_0\mathcal{H}}\mathbf{e}_k$ is a scalar multiple of $\mathbf{e}_j$ (or, equivalently, if $e^{it_0\mathcal{H}}\mathbf{e}_j$ is a scalar multiple of $\mathbf{e}_k$). 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 such that

$$|\mathbf{e}_j^T e^{it\mathcal{H}}\mathbf{e}_k|^2 \geq 1 - \varepsilon.$$

3. Hadamard-diagonalizable graphs with PST

The following theorem originally appeared in [4], restricted to the case of unweighted graphs. The following version instead allows for arbitrary integer edge weights. Although its proof is almost identical to its unweighted version, we include it here for completeness.

Theorem 1. [4] *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 0. Choose a non-zero eigenvalue λ of the Laplacian matrix L associated to G; the corresponding column of the Hadamard matrix that diagonalizes L is an eigenvector corresponding to λ. 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 λ. By applying some permutation operations, we find

$$\begin{bmatrix} L_1 + X_1 & -R \\ -R^* & L_2 + X_2 \end{bmatrix} \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix} = \lambda \begin{bmatrix} \mathbf{1} \\ -\mathbf{1} \end{bmatrix},$$

for some matrices X_1, X_2, and R (necessarily X_1, X_2 are diagonal).

As in [4], we arrive at the equality $2X_1\mathbf{1} = 2X_2\mathbf{1} = \lambda\mathbf{1}$. Since G is integer-weighted, then it follows that all eigenvalues are even integers, and the result follows. $\square$

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 $t_0 = \pi/2$.

Theorem 2. *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 $\lambda_1, \cdots, \lambda_n$, so that $LHe_j = \lambda_j He_j, j = 1, \dots, n$. Then G has PST from vertex j to vertex k at time $t_0 = \pi/2$ if and only if for each $\ell = 1, \cdots, n$, $\lambda_\ell \equiv 1 - h_{j\ell}h_{k\ell} \mod 4$.*

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

$$H^Te^{i(\pi/2)\Lambda}\mathbf{e}_j = H^T\mathbf{e}_k. \tag{1}$$

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 $\ell = 1, \cdots, n$, 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. □

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 $e^{itL} = e^{ita(\frac{1}{a}L)}$ 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 PST graphs: for example, if G has PST at $\pi/2$, and we are given the graph $2G$, we know that $2G$ has PST at $\pi/4$.

It is worth noting that Theorem 2 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 Λ 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 $t_0 = \pi/2$.

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 $G \vee G$ of G with itself is diagonalizable by the Hadamard $\begin{bmatrix} H & H \\ H & -H \end{bmatrix}$, 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 $G \vee G$ are diagonalizable follows from Lemma 7 in [4]. If we denote the eigenvalues of the Laplacian of G by $\lambda_1 = 0, \lambda_2, \cdots, \lambda_n$, then from Theorem 2 we know that for $\ell = 1, \cdots, n$, $\lambda_\ell \equiv 1 - h_{j\ell}h_{k\ell} \mod 4$. Therefore the eigenvalues $0, n - \lambda_2, \ldots, n - \lambda_n$ of G^c satisfy $(n - \lambda_\ell) \equiv -(1 - h_{j\ell}h_{k\ell}) \equiv 1 - h_{j\ell}h_{k\ell} \mod 4$, since $1 - h_{j\ell}h_{k\ell}$ is either 0 or $2 \bmod 4$ and n must be a multiple of 4 in order for a Hadamard of order n to exist.

Again from Theorem 2, we then know that G^c has PST from vertex j to k at time $\pi/2$. Thus $G \vee G = (G^c + G^c)^c$ 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 its eigenvalues are obtained from those of G by adding numbers congruent to $0 \bmod 4$.

4. Creation of New Hadamard-Diagonalizable Graphs with PST

We now introduce a new operation on graphs that, much like the union, join, and Cartesian product, can be used to construct new graphs with PST from old ones. Suppose that G_1 and G_2 are two weighted graphs that are both diagonalizable by a Hadamard matrix H 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 $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ 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 unweighted case (i.e., when $w_1 = w_2 = 1$), we denote the merge simply by $G_1 \odot G_2$.

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 $G_1 \,{}_{w_1}\!\odot_{w_2} G_2$ has twice as many vertices, which we label $\{1, \ldots, 2n\}$. Furthermore, if G_1 has edge (j,k) with weight w_{jk} then $G_1 \,{}_{w_1}\!\odot_{w_2} G_2$ 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 $G_1 \,{}_{w_1}\!\odot_{w_2} G_2$ has edge $(j, n+k)$ and $(k, n+j)$ with weight $w_2 w_{jk}$. See Figure 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,

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

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

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 scenaries.

Theorem 3. *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 $G_1 \,{}_{w_1}\!\odot_{w_2} G_2$ 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 $t_0 = \pi/2$;*

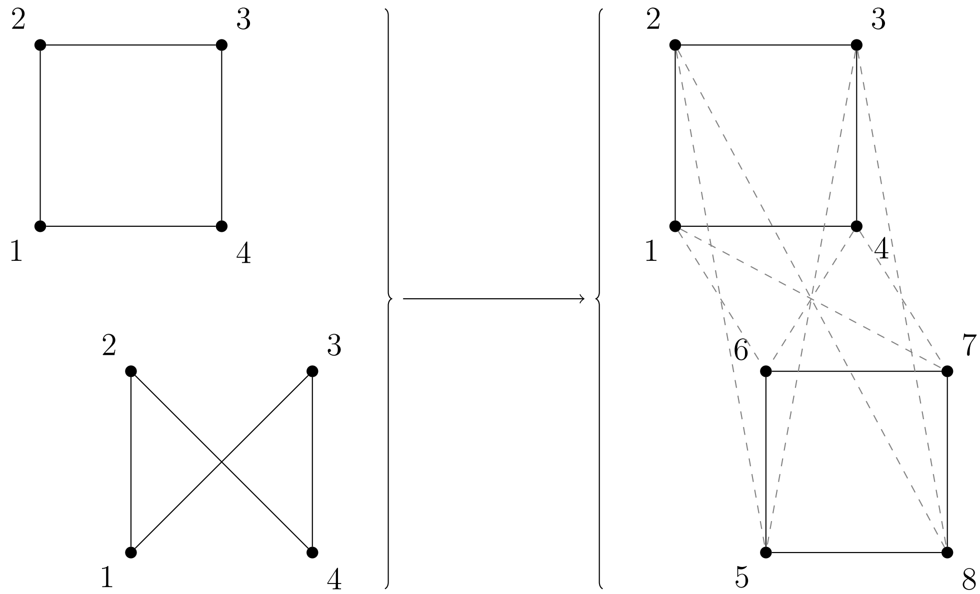

FIGURE 1. A depiction of two Hadamard-diagonalizable graphs (left) and their merge (right). The new graph has two copies of the original vertex set, and there is now an edge (j, k) and $(n + j, n + k)$ if and only if G_1 (top left) had edge (j, k), and there is an edge $(j, n + k)$ if and only if G_2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

(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 G_1, G_2 by Λ_1, Λ_2, respectively, so that $L_j = \frac{1}{n} H \Lambda_j H^T$, $j = 1, 2$. Let the Laplacian of $G_1 \;{}_{w_1}\!\odot_{w_2} G_2$ be $L_3 = \begin{bmatrix} w_1L_1 + w_2d_2I & -w_2A_2 \\ -w_2A_2 & w_1L_1 + w_2d_2I \end{bmatrix}$. Then

$$L_3 = \frac{1}{2n}\begin{bmatrix} H & H \\ H & -H \end{bmatrix}\begin{bmatrix} w_1\Lambda_1 + w_2\Lambda_2 & 0 \\ 0 & w_1\Lambda_1 - w_2\Lambda_2 + 2w_2d_2I \end{bmatrix}\begin{bmatrix} H & H \\ H & -H \end{bmatrix}^T.$$

Denote the eigenvalues of L_1, L_2 by $\lambda_\ell^{(1)}, \lambda_\ell^{(2)}, \ell = 1, \cdots, n$, respectively.

(1) Suppose that $p, q \in \{1, \cdots, n\}$ and L_3 has PST from p to q. Then for each $\ell = 1, \cdots, n$, $w_1\lambda_\ell^{(1)} + w_2\lambda_\ell^{(2)} \equiv (1 - h_{p\ell}h_{q\ell}) \mod 4$ and $w_1\lambda_\ell^{(1)} - w_2\lambda_\ell^{(2)} + 2w_2d_2 \equiv (1 - h_{p\ell}h_{q\ell}) \mod 4$. In particular, $2w_2d_2 \equiv 0 \mod 4$, i.e., w_2d_2 is even. Note that if w_1 and w_2 are both even, then $h_{p\ell}h_{q\ell} = 1$ for $\ell = 1, \cdots, n$, which is impossible.

If w_1 is odd and w_2 is even, then $w_1\lambda_\ell^{(1)} + w_2\lambda_\ell^{(2)} \equiv \lambda_\ell^{(1)} \mod 4$, so that $\lambda_\ell^{(1)} \equiv (1 - h_{p\ell}h_{q\ell}) \mod 4$, $\ell = 1, \cdots, n$. 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 $w_1\lambda_\ell^{(1)} + w_2\lambda_\ell^{(2)} \equiv \lambda_\ell^{(1)} + \lambda_\ell^{(2)} \equiv (1 - h_{p\ell}h_{q\ell}) \mod 4$, $\ell = 1, \cdots, n$. We deduce that $L_1 + L_2$ has PST from p to q.

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

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

$$w_1\lambda_\ell^{(1)} + w_2\lambda_\ell^{(2)} \equiv (1 - h_{p\ell}h_{\hat{q}\ell}) \mod 4, \text{ and} \tag{2}$$
$$w_1\lambda_\ell^{(1)} - w_2\lambda_\ell^{(2)} + 2w_2d_2 \equiv (1 + h_{p\ell}h_{\hat{q}\ell}) \mod 4. \tag{3}$$

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 $\lambda_\ell^{(2)} \equiv (1 - h_{p\ell}h_{\hat{q}\ell}) \mod 4$, $\ell = 1, \cdots, n$, 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 $\lambda_\ell^{(1)} + \lambda_\ell^{(2)} \equiv (1 - h_{p\ell}h_{\hat{q}\ell}) \mod 4$, $\ell = 1, \cdots, n$, which shows that the integer-weighted graph with Laplacian $L_1 + L_2$ has PST from p to $\hat{q}$.

The converses are straightforward. □

Note that when both w_1 and w_2 are even, the graph $G_1 \;{}_{w_1}\!\odot_{w_2} G_2$ 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 $w_j = 2^{r_j}.b_j$ (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 $\frac{1}{2^r}L_3$ at time $\pi/2$ can be determined according to the above theorem. In the case that PST occurs, the graph $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ would then have PST at time $\pi/2^{r+1}$ by Remark 1.

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 3. Similarly, $G_2 \odot G_1$ has PST from vertex p to q if d_2 is even (Case 1(b)), and it has PST from vertex p to $q + 2^m$ if d_2 is odd (Case 3(b)).

The following corollary to Theorem 3 provides an instance where the statement of the theorem simplifies considerably, and generalizes the known fact that the unweighted hypercube graph has PST.

Corollary 1. *Suppose $w_1, w_2, \ldots, w_n$ are integers, exactly d of which are odd. Then the weighted hypercube $C_n := (w_1K_2)\Box(w_2K_2)\Box\cdots\Box(w_nK_2)$ exhibits perfect state transfer at time $t_0 = \pi/2$ between every pair of vertices that are a distance of d from each other.*

Proof. We prove the result by induction. For the base case, we simply note that it is straightforward to verify that the weighted 1-cube w_1K_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 3 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 $G_1\ {}_1\!\odot_{w_{n+1}} G_2$ is exactly the weighted $(n+1)$-cube $C_{n+1} = (w_1K_2)\Box(w_2K_2)\Box\cdots\Box(w_{n+1}K_2)$, so condition 1(a) of the theorem tells us that if w_{n+1} is even then C_{n+1} 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 3 says that C_{n+1} 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). This completes the inductive step and the proof. $\Box$

Example 1. From Lemma 9 and Proposition 10 of [4], 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 be the graph whose Laplacian is

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

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

$$H = \begin{bmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 \\ 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 & 1 \\ 1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & 1 & 1 & 1 & -1 & -1 & -1 & 1 & -1 & -1 \end{bmatrix}$$

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 $w_2 = 2$. Then Case 1(a) of Theorem 3 tells us that $G_1 \;{}_5{\odot}_2\; G_2$ 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, 54, 64, 64, 64, 54, 54, 54, 44, 54, 44, 50, 60, 50, 60, 60, 60, 50, 50, 50, 40, 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 $t_0 = \pi/2$.

With the merge operation in hand, we can now show that there exist Hadamard-diagonalizable graphs with PST of almost any regularity. Specifically, for each $k \geq 3$ and each d with $k+1 \leq d \leq 2^k-2$, there is a d-regular unweighted, connected, and non-bipartite graph on 2^k vertices that is diagonalizable by the standard Hadamard matrix and has PST at time $t_0 = \pi/2$. Note that a (2^k-1)-regular unweighted graph on 2^k vertices is a complete graph, which is known not to have PST, so the upper bound on d is the best possible. Also recall that it is known that the k-hypercube graph is regular with degree k and has PST at time $t_0 = \pi/2$, and it is straightforward to check that it is Hadamard-diagonalizable, but because it is bipartite the following theorem does not apply to it.

Theorem 4. *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*
(3) *has PST between distinct vertices at time $t_0 = \pi/2$.*

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 $(K_{2,2}\square K_2)^c$, $(K_{2,2}+K_{2,2})^c$ and $(K_2+K_2+K_2+K_2)^c$ are 4-, 5-, and 6-regular graphs 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 2 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 $G_{k,d-1}\square K_2$. 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_{2^r} 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 $G_{k,d'}^{(r)} = G_r \odot G_{k,d'}$ 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 2, it also has PST between a pair of distinct vertices. It is regular of degree $d' + 2^r - 1$. Also in the notation of Theorem 3, $-\Lambda_2 + 2d'I$ 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 $G_{k+1,d'+2^r-1}$.

Thus we have produced the desired graphs whose degrees fall in the set

$$[k+2, 2^k - 1] \cup \bigcup_{r=2}^{k} [k + 2^r, 2^k + 2^r - 3]. \tag{4}$$

For $k = 3$ that 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 $G^c \vee G^c$ 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 $[k + 2, 2^{k+1} - 3]$.

□

Remark 3. Note that for $2^k + 1 \leq d \leq 2^{k+1} - 2$, 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 $G \vee G$ 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, $G \vee G$ 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 lcm be the least common multiple of the denominators of its edge weights, and gcd be the greatest common divisor of all the new integer edge weights $lcm \cdot w(j,k)$. Then G_1 has PST at time $t_1 = \frac{lcm}{gcd} \cdot \pi/2$ if and only if the integer-weighted Hadamard-diagonalizable graph G_2 with Laplacian $L_2 = \frac{lcm}{gcd} L_1$ 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

$$|\mathbf{e}_j^T e^{it_0 L_2}\mathbf{e}_k|^2 = |\mathbf{e}_j^T e^{it_0 \frac{lcm}{gcd} L_1}\mathbf{e}_k|^2 = |\mathbf{e}_j^T e^{it_1 L_1}\mathbf{e}_k|^2, \tag{5}$$

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 will neither be Hadamard-diagonalizable nor will it 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 $G_1 \; {}_{w_1}\!\odot_{w_2} G_2$ is irrational. Before giving the theorem, we recall the following result about approximating an irrational real number with rational numbers.

Theorem 5 ([18])**.** *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 $[o, e]$, $[e, o]$, and $[o, o]$, such that the inequality $|w - u/v| < 1/v^2$ holds.*

For the graph $G_1 \; {}_{w_1}\!\odot_{w_2} G_2$, we say it has parameters $[w_1, w_2, d_2]$, where as in Theorem 3, d_2 denotes the degree of G_2. In particular, if w_1, w_2, and d_2 are all odd integers, we say the graph $G_1 \; {}_{w_1}\!\odot_{w_2} G_2$ has type $[o, o, o]$. We will denote the set of irrational numbers by $\overline{\mathbb{Q}}$.

Theorem 6. *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 an integer and the other is irrational, and suppose that $p, q \in \{1, \ldots, n\}$. Then the weighted graph $G_1 \; {}_{w_1}\!\odot_{w_2} G_2$ has PGST as stated in the following cases.*

(1) $w_1 \in \mathbb{Z}, w_2 \in \overline{\mathbb{Q}}$.

(a) *Suppose that G_1 has PST from p to q at time $\pi/2$. If w_1 is odd, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to q and from $p+n$ to $q+n$.*

(b) *Suppose that G_2 has PST from p to q at time $\pi/2$. If d_2 is even, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to q and from $p+n$ to $q+n$. If d_2 is odd, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to $q+n$ and from q to $p+n$.*

(c) *Suppose that $L_1 + L_2$ has PST from p to q at time $\pi/2$, and w_1 is odd. If d_2 is even, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to q and from $p + n$ to $q + n$. If d_2 is odd, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to $q + n$ and from q to $p + n$.*

(2) $w_1 \in \overline{\mathbb{Q}}, w_2 \in \mathbb{Z}$.

(a) *If G_1 has PST from p to q at time $\pi/2$, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to q and from $p + n$ to $q + n$.*

(b) *Suppose that G_2 has PST from p to q at time $\pi/2$, and that w_2 is odd. If d_2 is even, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to q and $p + n$ to $q + n$. Further if d_2 is odd, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to $q + n$ and q to $p + n$.*

(c) *Suppose that $L_1 + L_2$ has PST from p to q at time $\pi/2$ and that w_2 is odd. If d_2 is even then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to q and $p+n$ to $q+n$. If d_2 is odd, then $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ has PGST from p to $q + n$ and q to $p + n$.*

Proof. As in the proof of Theorem 3, without loss of generality we assume that H is a normalized Hadamard matrix. Assume w_1 is an integer, and w_2 is irrational. We approach w_2 with fractions u/v such that $|w_2 - u/v| < 1/v^2$. We denote the graph $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ as G_3. For each such pair of u, v, we denote the graph $G_1\ {}_{w_1}\!\odot_{u/v} G_2$ as G_4, and the graph $G_1\ {}_{0}\!\odot_{w_2-u/v} G_2$ 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_3, G_4 and G_5 as L_3, L_4, and L_5, respectively. Now consider the integer-weighted graph $G_4' = G_1\ {}_{vw_1}\!\odot_u G_2$, then its Laplacian is vL_4 and has parameters $[vw_1, u, d_2]$.

Case 1: w_1 is odd.

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 3 we know, if G_2 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(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 3 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 3 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 $[o,o,e]$. From Theorem 3 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 3 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)).

Case 2: w_1 is even.

If $[u,v]$ is of type $[o,e]$ or $[o,o]$ and d_2 is even, the graph G_4' is of type $[e,o,e]$. From Theorem 3 we know that if G_2 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(b), 2(b)). If $[u,v]$ is of type $[o,e]$ or $[o,o]$ and d_2 is odd, the graph G_4' is of type $[e,o,o]$. From Theorem 3 we know that if G_2 has PST 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)).

Similarly we can get the results when w_1 is real irrational and w_2 is an integer. For all the above cases, G_4 has PST at time $t_0 = v\pi/2$. Next,we recall the following result from [13, 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

$$(6)\qquad 1 - |\mathbf{e}_j^T e^{it_0(L+L_0)}\mathbf{e}_k|^2 \;\leq\; 2\|t_0L_0\| + \|t_0L_0\|^2 - \|t_0L_0\|^3.$$

Now we can see G_3 as a graph with PST at time t_0. Then the fidelity of state transfer of G_3 between the corresponding pair of vertices satisfies

$$\begin{aligned} |\mathbf{e}_j^T e^{it_0L_3}\mathbf{e}_k|^2 &\geq 1 - 2\|t_0L_5\| - \|t_0L_5\|^2 + \|t_0L_5\|^3 \\ &\geq 1 - 2bn\pi/(2v) - (bn\pi/(2v))^2 + (bn\pi/(2v))^3, \end{aligned}$$

where b is the maximum edge weight in G_2. Since there are infinitely such integers v, the expression at the end of the above inequality can be made as small as possible. □

Example 2. Consider the unweighted graphs G_1, G_2 with the following Laplacian matrices:

$$L_1 = \begin{bmatrix} 3 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & 3 & 0 & -1 & 0 & -1 & 0 & 0 \\ -1 & 0 & 3 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & -1 & 3 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 3 & -1 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 3 & 0 & -1 \\ 0 & 0 & -1 & 0 & -1 & 0 & 3 & -1 \\ 0 & 0 & 0 & -1 & 0 & -1 & -1 & 3 \end{bmatrix}$$

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 is odd and $w_2 \in \overline{\mathbb{Q}}$, then $G_1 \;{}_{w_1}\!\odot_{w_2} G_2$ has the intriguing property that there is PGST between the pairs $(1,8),(1,14),(1,11),(9,16)$ (among others). Similarly if w_2 is odd and $w_1 \in \overline{\mathbb{Q}}$, then $G_1 \;{}_{w_1}\!\odot_{w_2} G_2$ has PGST between the pairs $(1,8),(1,14),(1,11),(9,16)$ (among others).

6. Optimality

6.1. **Timing Errors.** In [13], 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 give in the most general setting where no information is known about the graph in question. Suppose a graph G has PST at time t_0 and that there is a small perturbation so that the readout time is instead $t_0 + h$, where $|h| < \frac{\pi}{\lambda_n - \lambda_1}$, where λ_1 and λ_n are the smallest and largest eigenvalues, respectively, of the corresponding Laplacian. Decompose the Laplacian as $L = Q\Lambda Q^T$, where $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$ and Q is an orthogonal matrix of corresponding eigenvectors. If $\mathbf{q}_1 = (q_{11}, \ldots, q_{n1})^T$ is the first column of Q^T and $M = \operatorname{diag}(e^{ih\lambda_1}, \ldots, e^{ih\lambda_{2^n}})e^{i\theta}$, then

$$p(t_0) - p(t_0 + h) \;=\; 1 - |\mathbf{q}_1^T M \mathbf{q}_1|^2$$

where for any $s \in \mathbb{R}$,

$$|\mathbf{q}_1^T M \mathbf{q}_1| \;=\; \left| \sum_{j=1}^{n} q_{j1}^2 e^{ih(\lambda_j - s)} \right|. \tag{7}$$

Equation (7) was given in the proof of Theorem 2 in [13]. Here we have $Q = \frac{1}{\sqrt{n}} H$, where H is a Hadamard matrix, so we can say more. Indeed, choosing $s = 0$ yields

$$|\mathbf{q}_1^T M \mathbf{q}_1| \;=\; \frac{1}{n} \left| \sum_{j=1}^{n} e^{ih\lambda_j} \right| \tag{8}$$

This suggests that, in order to find a lower bound for $|\mathbf{q}_1^T M \mathbf{q}_1|$ (and thus an upper bound for $p(t_0) - p(t_0 + h)$), the goal should be to make the numbers $e^{ih\lambda_j}$ as closely-spaced on the complex unit circle as possible. This agrees with the known fact that minimizing the spectral spread has the effecting of maximizing the bound for the fidelity of state transfer due to timing errors [15]. 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 7. *Let G be a simple, connected, unweighted r-regular graph with perfect state transfer on n vertices, and suppose 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 $\operatorname{Tr}(L^k)$ ($k \geq 0$ is an integer) in two different ways. First, if $\lambda_1, \ldots, \lambda_n$ are the eigenvalues of L then $\operatorname{Tr}(L^k) = \sum_{j=1}^{n} \lambda_j^k$, 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 $\operatorname{Tr}(L) = rn - \operatorname{Tr}(A)$ and $\operatorname{Tr}(L^2) = r^2 n - 2r\operatorname{Tr}(A) + \operatorname{Tr}(A^2)$. Since A is simple, we know that $\operatorname{Tr}(A) = 0$ and it is straightforward to compute

$\mathrm{Tr}(A^2) = rn$. 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_λ denote the number of eigenvalues of L equal to λ (with the convention that if λ is not an eigenvalue, then $c_\lambda = 0$), then these equations tell us that

$$\sum_{j=1}^{r} (2j)c_{2j} = rn \quad \text{and} \quad \sum_{j=1}^{r} (2j)^2 c_{2j} = rn(r+1). \tag{9}$$

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 $n = 8 = 2^r$.

For the $r = 4$ case, we use the Equations (9) 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 $\mathrm{Tr}(L^3)$ in two different ways (similar to at the start of the proof): $\mathrm{Tr}(L^3) = \sum_{j=1}^{n} \lambda_j^3 = r^3 n - 3r^2 \mathrm{Tr}(A) + 3r\mathrm{Tr}(A^2) - \mathrm{Tr}(A^3) = r^3 n + 3r^2 n - \mathrm{Tr}(A^3)$. Since $\mathrm{Tr}(A^3) \geq 0$ 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 7 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 7 to the $r = 5$ case, we might try computing $\mathrm{Tr}(L^4)$ in two different ways. However, we then end up with an equation involving both $-\mathrm{Tr}(A^3)$ and $+\mathrm{Tr}(A^4)$, and it is not clear how to bound such a quantity.

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