COMBINATORIAL AND ALGEBRAIC ASPECTS OF QUANTUM STATE TRANSFER

by

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Abstract

Reliably transferring a quantum state from one location to another, as well as generating entangled states, are important tasks to achieve in quantum spin systems. The fidelity or probability of state transfer is a number between 0 and 1 that measures the closeness of two quantum states.

Fidelity is used to determine the accuracy of quantum state transfer. There are several interesting phenomena of quantum state transfer defined via fidelity: perfect state transfer, pretty good state transfer, and fractional revival.

This thesis contains results about the perfect state transfer property of some special classes of graphs, including Hadamard diagonalizable graphs, weighted paths with loops, as well as switched and partially switched hypercubes. A correspondence between the class of graphs that are diagonalizable by a standard Hadamard matrix and the class of cubelike graphs is given. Sensitivity of fidelity to errors when perfect state transfer occurs is analysed: if a system admits perfect state transfer at some time t, bounds on fidelity of state transfer at $t + h$ for very small h are given, as well as bounds on fidelity of a slightly perturbed system at time t. Finally, Laplacian fractional revival on graphs is considered;

in particular the thesis contains a characterization of threshold graphs that admit Laplacian fractional revival.

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List of symbols

G	an undirected weighted or unweighted graph with or without loops
$\hat{P}$	the normalized characteristic matrix of a partition of a graph
G/π	the quotient of G with respect to an equitable partition π of G
$\widehat{G/\pi}$	the symmetrized quotient of G with respect to an equitable partition π of G
G^c	the complement of G
$G_1 \cup G_2$	the union of two graphs G_1 and G_2
$G_1 \vee G_2$	the join of two graphs G_1 and G_2
$G_1 \square G_2$	the Cartesian product of two graphs G_1 and G_2
$G_1 \; {}_{w_1}\!\odot_{w_2} G_2$	the merge of graphs G_1 and G_2 with respects to the weights w_1 and w_2
K_n	the complete graph on n vertices
O_n	the empty graph on n vertices
$A(G)$	the adjacency matrix of G
$L(G)$	the Laplacian matrix of G

M_n	the set of all $n \times n$ matrices over $\mathbb{C}$
I_n	the identity matrix of size n
$0_{m,n}$	the zero matrix of size $m \times n$
$J_{m,n}$	the all-ones matrix of size $m \times n$
J_n	the all-ones matrix of size $n \times n$
$J_{(n)}$	the all-ones matrix of size $2^n \times 2^n$
$A \otimes B$	the tensor product of two matrices A and B
$\sigma(A)$	the spectrum of A
$\rho(A)$	the spectral radius of A
$p_{j,k}(t)$	the fidelity of state transfer from vertex j to vertex k at time t
x^T	the transpose of x
x^*	the conjugate transpose of x
A^*	the conjugate transpose of a matrix A
$\|x\|_2$	the Euclidean norm of x
$\|A\|_F$	the Frobenius norm of A
$\|\|\|A\|\|\|_2$	the spectral norm of A
$\mathrm{Tr}(A)$	the trace of a square matrix A
$\mathbb{N}$	the set of all positive integers
$\|a\|$	the modulus of $a \in \mathbb{C}$
$\mathbf{1}_n$	the all-ones vector in $\mathbb{C}^n$
$\mathbf{0}_n$	the all-zeros vector in $\mathbb{C}^n$
$e_1, \ldots, e_n$	the standard basis vectors of the vector space $\mathbb{C}^n$

Chapter 1

Introduction

1.1 Physics motivation

In this section, we briefly mention the motivation stemming from physics, as well as related physics definitions. Physical lab experiments implementing quantum state transfer protocols are described in e.g. [28, 71]. The work herein describes the notion of quantum state transfer from a mathematical perspective; this theoretical research plays an important role in quantum information transfer. From Section 1.2 onward, the corresponding definitions and results are stated in a mathematical way.

A spin has two computational basis states: $e_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $e_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$, they form a basis of the vector space $\mathbb{C}^2$, and the general state φ of a spin can be represented as a linear superposition of the two basis vectors: $\varphi = \alpha e_1 + \beta e_2$ with $|\alpha|^2 + |\beta|^2 = 1$. Other orthonormal basis states can also be used. We say that two quantum states $\varphi_1 = \alpha_1 e_1 + \beta_1 e_2$ and

$\varphi_2 = \alpha_2 e_1 + \beta_2 e_2$ are identical up to complex modulus if $|\alpha_1| = |\alpha_2|$ and $|\beta_1| = |\beta_2|$. A quantum system consisting of two spins has four orthonormal basis states: $e_1, e_2, e_3, e_4 \in \mathbb{C}^4$, and the general state φ of the system can be written as a linear combination of these four states: $\varphi = \alpha_1 e_1 + \alpha_2 e_2 + \alpha_3 e_3 + \alpha_4 e_4$ with $|\alpha_1|^2 + |\alpha_2|^2 + |\alpha_3|^2 + |\alpha_4|^2 = 1$. In general, the state of a quantum spin system with n spins that are usually interacting with each other can be represented by a unit vector $\varphi \in \mathbb{C}^{2^n}$.

The Hamiltonian $\mathcal{H}$ of a quantum system consisting of n spins is a Hermitian operator on $\mathbb{C}^{2^n}$; its spectrum is the set of possible outcomes when one measures the total energy of the system. Due to its own dynamics, the system evolves according to the Schrödinger equation [83]:

$$i\hbar \frac{d}{dt}\varphi_t = \mathcal{H}\varphi_t, \tag{1.1}$$

where φ_t is the state vector and $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant.

Transferring a quantum state from one location to another reliably, as well as generating entangled states, are important tasks to achieve in quantum spin systems. The *fidelity or probability of state transfer* measures the closeness of two quantum states, and it is a number between 0 and 1. By measuring the closeness of the state of spin v at time $t = t_0$ to the state of spin u at time $t = 0$, fidelity is used to determine the accuracy of quantum state transfer from spin u to spin v. If this fidelity is 1, it means that the state read out by the receiver at spin v at time t_0 is, with probability equal to one, identical up to complex modulus to the input state of the sender at time $t = 0$, and we say there is *perfect state transfer (PST)* between the two spins at time $t = t_0$. If for some two spins u and v, there is a time sequence $\{t_m\}_{m\geq 1}$ such that the fidelity of state transfer between u and v at time t_m approaches 1 as $m \to \infty$, we say there is *pretty good state transfer (PGST)* between u and v.

If there is a time t such that for any two spins u and v of the system, the fidelity of state transfer from u to v is a fixed number (independent of u and v), then we say that there is *uniform mixing* on the quantum spin system at time t. If there is a time t, and two distinct spins u and v, such that the fidelity from u to any other spin w (i.e., $w \neq u, v$) is 0, and that the fidelity of state transfer from u to v is non-zero, then we say that there is *fractional revival (FR)* between the two spins u and v.

Throughout the thesis, for a quantum system of n spins, we focus on the single excitation subspace: an invariant n-subspace (spanned by the standard basis $e_1, \ldots, e_n \in \mathbb{C}^n$) of the full 2^n-dimensional Hilbert space $\mathbb{C}^{2^n}$. In this case, the Hamiltonian reduces to a real symmetric operator on $\mathbb{C}^n$ [31].

We can model a quantum spin system by an undirected weighted graph: assign a vertex to each spin, and connect two vertices with an edge if and only if the corresponding spins interact with each other in the quantum system, with the corresponding edge weight equal to the interaction strength between the two spins. Recently, research has also been done on PST, PGST and FR in quantum systems (in particular, in quantum spin chains) with added potentials on their spins, which can be modelled by undirected weighted graphs with loops. In this work, we use the terms “an undirected weighted graph” and “a quantum system” interchangeably.

1.2 Basic notation

In this thesis, we focus on undirected weighted graphs, and use the term *graph* to refer to a simple graph, and *graph with loops* to refer to a multigraph that allows for loops but not multiple edges. For more information on the basics of graph theory, see [49, 88].

A graph G consists of a vertex set $V(G)$ and an edge set $E(G)$, where an edge is an unordered pair of distinct vertices of G. If $\{u, v\}$ is an edge, we say that u and v are *adjacent* or that u and v are *neighbours*.

A graph with loops G consists of a vertex set $V(G)$ and an edge set $E(G)$, where an edge is an unordered pair of vertices (not necessarily distinct) of G. An edge of the form $\{u, u\}$ is called a *loop* of G, and in this case we say that u is adjacent to itself.

The *degree* $\deg(v)$ of vertex v in an undirected graph (with or without loops) is the number of edges incident to it, where each loop contributes 2 to its degree.

A *weighted graph (with or without loops)* is a graph (with or without loops, respectively) with (real) numerical labels/weights on the edges; the label on edge $\{u, v\}$ is called the *weight* of the edge. For a weighted graph with loops, the label on a loop is called the weight of the loop.

The *degree* $\deg(v)$ of vertex v in an undirected weighted graph (with or without loops) is the sum of the weights of edges incident to it, where the weight of a loop at vertex v contributes twice to the degree of that vertex: that is, $\deg(v) = \sum_{u \neq v} w_{u,v} + 2w_{v,v}$, where $w_{u,v}$ denotes the weight of the edge $\{u, v\}$.

A graph is called *complete* if any two (distinct) vertices are adjacent, and the complete graph on n vertices is denoted by K_n. A graph with no edges (but at least one vertex) is called *empty*. An empty graph on n vertices is denoted by O_n. A graph G is called *bipartite* if its vertex set can be partitioned into two parts V_1 and V_2 such that every edge has one end in V_1 and one in V_2.

A *subgraph* of a graph G is a graph Y such that $V(Y) \subseteq V(G)$, and $E(Y) \subseteq E(G)$. If $V(Y) = V(G)$, we call Y a *spanning subgraph* of G. A subgraph Y of G is an *induced subgraph* if two vertices of $V(Y)$ are adjacent in Y if and only if they are adjacent in G. A set of vertices that induces an empty subgraph is called an *independent set*.

A *path* of length r from vertex u to vertex v in a graph is a sequence of $r+1$ distinct vertices starting with u and ending with v such that any two consecutive vertices are adjacent. If between any two vertices, there is a path, then G is *connected*, otherwise G is *disconnected*. The *distance* $d_G(u, v)$ is the length of a shortest path from u to v. Note that the distance between two vertices is usually considered ∞ if there is no path between them. The *diameter* of a connected graph G is $\max\{d_G(u, v) | u, v \in V(G), u \neq v\}$.

A *cycle* is a connected graph where every vertex has exactly two neighbours. The phrase "a cycle in a graph" refers to a subgraph of G that is a cycle. A connected spanning subgraph with no cycles is called a *spanning tree*.

Two graphs G and Y are *isomorphic* if there is a bijection ϕ from $V(G)$ to $V(Y)$ such that u is adjacent to v in G if and only if $\phi(u)$ is adjacent to $\phi(v)$ in Y. We say that ϕ is an *isomorphism* from G to Y. An isomorphism from a graph G to itself is called an *automorphism* of G. A graph G is *vertex-transitive* if and only if for any two vertices u

and v of G, there is a graph automorphism ϕ of G such that $\phi(u) = v$.

A *directed graph (digraph)* G consists of a vertex set $V(G)$ and an arc set $E(G)$, where an *arc*, or a *directed edge*, is an ordered pair of distinct vertices.

Analogous definitions of subgraphs etc. can be made for a graph with loops.

Throughout, we use $e_1, \ldots, e_n$ to denote the standard basis vectors in the n-dimensional vector space, where for each $j = 1, \ldots, n$, $e_j = [0, \ldots, 0, 1, 0, \ldots, 0]^T$ (1 is in the j-th position), we use $J_{m,n}$ to denote the all ones matrix of size $m \times n$, we use $\mathbf{1}_n$ to denote the all ones vector of dimension n, and we use I_n to denote the identity matrix of size $n \times n$. We denote a $m \times n$ zero matrix by $0_{m,n}$ and the zero vector in $\mathbb{C}^n$ by $\mathbf{0}_n$. The set of all $n \times n$ matrices is denoted by M_n.

1.3 Mathematical setup and definitions

Assume that G is a weighted graph with or without loops on n vertices, and label the vertices of G by integers from 1 to n. The *adjacency matrix* $A(G) = [a_{j,k}]_{1 \le j,k \le n}$ of G is the $n \times n$ matrix

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

where $w_{j,k}$ is the *weight* of the edge between vertices j and k.

If G is an unweighted graph, or simply a graph, then its adjacency matrix is defined as above, with all (nonzero) weights being equal to 1.

For a weighted or unweighted graph G with or without loops, its *degree matrix* $D(G)$

is a diagonal matrix with its j-th diagonal entry equal to $\deg(j)$, the degree of vertex j. The *Laplacian matrix* of G is defined as $L(G) = D(G) - A(G)$, where $A(G)$ is the adjacency matrix, and $D(G)$ is the degree matrix associated to G. Note that both $A(G)$ and $L(G)$ are symmetric matrices. Furthermore, the Laplacian matrix $L(G)$ of a weighted or unweighted graph without loops has 0 as its smallest eigenvalue, with $\mathbf{1}$, the all 1s vector, as an associated eigenvector. For a simple graph G, the multiplicity of the eigenvalue 0 of $L(G)$ corresponds to the number of connected components of G. Note that if G has loops, then $L(G)$ might not have 0 as an eigenvalue – for example, if $A(G) = \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix}$ and $L(G) = \begin{bmatrix} 2 & -1 \\ -1 & 0 \end{bmatrix}$.

With the adjacency matrix and Laplacian matrix at hand, we can define two relations on the vertex set of a weighted or unweighted graph. Assume that G is a weighted or unweighted graph with or without loops. For any vertex w of G, denote the induced subgraph of G on $V(G)\backslash\{w\}$ by $G\backslash w$. For two distinct vertices u and v of G, we say that u and v are *cospectral* with respect to the adjacency matrix if $A(G\backslash u)$ and $A(G\backslash v)$ have the same characteristic polynomial. Similarly we can define cospectral vertices with respect to the Laplacian matrix if we replace all the adjacency matrices by the corresponding Laplacian matrices in the above definition.

For any weighted or unweighted graph with or without loops, there is a unique adjacency matrix and a unique Laplacian matrix associated to it. Conversely, given a square matrix $B = [b_{j,k}]_{1\leq j,k\leq n}$ of size n, we can also associate a unique graph (possibly with loops) (if B is symmetric) or a unique digraph (if B is not symmetric) to B. Assume the rows and columns of B are labelled by $1, \dots, n$, and assign one vertex to each of the n indices. If B is symmetric, we connect vertices j and k in the graph if $b_{j,k} \neq 0$; if B is not symmetric, we draw an arc from vertex j to vertex k in the digraph if $b_{j,k} \neq 0$. The resulting graph (or digraph) is called the unweighted graph (or digraph) associated to the matrix B. Note that different square matrices might have the same unweighted graph (or digraph) with loops associated to them.

A weighted or unweighted graph with or without loops is *regular* if all its vertices have the same degree, that is, the degree matrix D is a scalar matrix (a scalar multiple of the identity matrix), and in this case, we simply call this scalar the *degree* of the graph.

The matrix exponential of a complex square matrix X, denoted by e^X or $exp(X)$, is given by the power series $e^X = \sum_{k=0}^{\infty} \frac{X^k}{k!}$, where X^0 is defined to be the identity matrix of the same size as X.

Proposition 1.3.1. [54, Proposition 2.3] *Let X and Y be $n \times n$ complex matrices, the matrix exponential satisfies the following properties.*

- $e^0 = I$,
- $e^{X^T} = (e^X)^T$,
- $e^{X^*} = (e^X)^*$,
- *If Y is invertible, then* $e^{YXY^{-1}} = Ye^XY^{-1}$,
- *If $XY = YX$, then* $e^Xe^Y = e^{X+Y}$.

As mentioned in Section 1.1, the Hamiltonian of a system is an operator corresponding to the total energy of the system, and its spectrum is the set of all possible outcomes if one measures the total energy of the system. For the one-excitation subspace — the only situation we consider in this thesis — the Hamiltonian of a system with n spins reduces to a real symmetric $n \times n$ matrix. There are two common types of dynamics for a quantum system: XY dynamics and Heisenberg dynamics. The Hamiltonians corresponding to each dynamics are identified in Remark 1.3.2.

Remark 1.3.2. [31, 78] If the quantum system is governed by XY dynamics, then the adjacency matrix A of the underlying graph (with or without loops) serves as the Hamiltonian of the system, and if the system is governed by Heisenberg dynamics, then the Hamiltonian can be represented by the Laplacian matrix L of the graph (with or without loops).

Definition 1.3.3. *Let G be a weighted graph (with or without loops) with vertices labelled $1, 2, \ldots, n$, and let $\mathcal{H}$ denote its Hamiltonian (a real symmetric operator). Let $U(t) = e^{it\mathcal{H}}$. Then the* fidelity or probability *of quantum state transfer from vertex j to vertex k at time t is*

$$p_{j,k}(t) = |(U(t))_{j,k}|^2 = |e_j^T e^{it\mathcal{H}} e_k|^2. \tag{1.2}$$

Recall that for any real symmetric matrix M of size $n \times n$, there is a real orthogonal matrix $Q = [q_{j,k}]$ such that $Q^T M Q = \Lambda$ for some diagonal matrix $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$.

Then

$$|e_j^T e^{itM} e_k|^2 = |e_j^T e^{itQ\Lambda Q^T} e_k|^2 = |e_j^T Q e^{it\Lambda} Q^T e_k|^2 = |q_j^T e^{it\Lambda} q_k|^2 = |\sum_{\ell=1}^{n} e^{it\lambda_\ell} q_{j,\ell} q_{k,\ell}|^2, \tag{1.3}$$

where q_j denotes the j-th column of Q^T. Applying this to the Hamiltonian $\mathcal{H}$, we get a direct formula to calculate the fidelity of state transfer.

From the above definition we know that $U(t)$ is a complex symmetric matrix (since $\mathcal{H}$ is symmetric), therefore $p_{j,k}(t) = p_{k,j}(t)$ for any time t, that is, for any time t, the fidelity of state transfer from vertex j to vertex k is the same as the fidelity of state transfer from vertex k to vertex j. Also $U(t)^* U(t) = U(-t)U(t) = U(0) = I_n$ implies that $U(t)$ is a unitary matrix.

Proposition 1.3.4. *Let $\mathcal{H}$ be the Hamiltonian of a (weighted) graph G, and let $U(t) = e^{it\mathcal{H}}$. Then $U(t)$ is a unitary symmetric matrix.*

The above fact implies that each row and column of $U(t)$ has Euclidean norm 1, hence the square of the modulus of any entry of $U(t)$ — i.e., fidelity of state transfer — is a number between 0 and 1. The facts that for any fixed time t, $\sum_{k=1}^{n} p_{j,k}(t) = 1$ and that $p_{j,k}(t) \geq 0$ show that $p_{j,k}(t)$ can be interpreted as the probability that the state at vertex j at time 0 is transferred to vertex k at time t. In fact, for a given system and any time $t > 0$, the matrix of fidelities $[p_{j,k}(t)]_{1 \leq i,k \leq n}$ is a (symmetric) doubly stochastic matrix, and a discrete time random walk can be associated to it [82]. Based on fidelity, several phenomena about quantum systems have been defined in the literature. The most special case occurs when some fidelity equals to 1.

Definition 1.3.5. *Let G be a weighted graph on n vertices. If there is some time $t_0 > 0$ and a vertex j such that $p_{j,j}(t_0) = 1$, then we say that G is* periodic *at vertex j at time t_0. If there is some time t_1 and two distinct vertices j and k such that $p_{j,k}(t_1) = 1$, then we say that there is* perfect state transfer (PST) *from vertex j to vertex k at time t_1.*

If G admits perfect state transfer from vertex j to vertex k at time t_1, it means that, up to a phase factor, the state at vertex k at time $t = t_1$, is identical to the initial state we put at vertex j at time $t = 0$. Also note that if G admits perfect state transfer from j to k, then G is periodic at vertex j and k, as shown in the following proposition.

Proposition 1.3.6. *Let G be a (weighted) graph that admits perfect state transfer from vertex j to vertex k at time t_1. Then G is periodic at vertex j (and vertex k) at time $2t_1$.*

Proof. Relabel the vertices of G such that j and k are labelled 1 and 2, respectively. Then $U(t)$ is a block diagonal matrix, with the first block of the form $\begin{bmatrix} 0 & \alpha \\ \alpha & 0 \end{bmatrix}$ for some complex number α of modulus 1. Therefore $U(2t_1) = U(t_1)U(t_1)$ is also block diagonal with the first block equal to $\begin{bmatrix} \alpha^2 & 0 \\ 0 & \alpha^2 \end{bmatrix}$, from which we can see that G is periodic at the first two vertices at time $2t_1$. $\square$

Unfortunately, perfect state transfer is not always achievable for some given graph G; for example, it was found [31] that an unweighted path on n vertices admits PST only for $n = 2, 3$ under XY dynamics, and only for $n = 2$ under Heisenberg dynamics. Also in practice, to get fidelity 1, the state at vertex k has to be read out at the precise time t_1, but even with lab equipment calibrated to an arbitrary amount of precision, we might read out at time $t_1 + h$ for small h, for example, $h = \pm 0.00001$. Hence in reality, with a high chance, the fidelity of state transfer at a readout time is just very close to 1, but not precisely 1. The situation where there is no perfect state transfer, but the fidelity of state transfer between some pair of vertices can be very close to 1, is also of high importance.

Definition 1.3.7. *Let G be a weighted graph (with or without loops) on n vertices. If there are two distinct vertices j and k, and a time sequence $\{t_m\}$, such that the sequence $\{p_{j,k}(t_m)\}$ of fidelities of state transfer between vertices j and k approaches 1 as $m \to \infty$, then we say that there is* pretty good state transfer (PGST) *from vertex j to vertex k.*

Another way to generalize the definition of perfect state transfer is to consider the case where the fidelity of state transfer at some time $t = t_2$ from vertex j to any other vertex is 0 apart from some vertex $k \neq j$ and possibly vertex j itself. This means that the initial state placed at vertex j at time $t = 0$, is at time $t = t_2$ transferred back to vertex j with some probability $0 \leq p < 1$, and is transferred to another different fixed vertex k with probability $0 < 1 - p \leq 1$.

Definition 1.3.8. *Let G be a weighted graph (with or without loops) on n vertices. If there are a time t_2 and two distinct vertices j, k such that $p_{j,j}(t_2) + p_{j,k}(t_2) = 1$ with $p_{j,k}(t_2) \neq 0$, then we say there is* fractional revival (FR) *from vertex j to vertex k at time t_2. More generally, if there is a time t_3 and a proper subset $S \subset V(G)$ (with $|S| < n$), such that for any $j \in S$, $\ell \notin S$, $p_{j,\ell}(t_3) = 0$, and the unweighted graph associated to the submatrix $U(t_3)_{[S,S]}$ is connected, then we say there is* generalized fractional revival between vertices in S, *where* $U(t_3)_{[S,S]}$ *is the submatrix of entries that lie in the rows and columns of* $U(t_3)$ *indexed by elements in* S.

If $\mathcal{H} = A$ (or $\mathcal{H} = L$) and the system admits PST, PGST or FR, then we say that there is adjacency (or Laplacian, respectively) PST, PGST or FR, or say that the system admits adjacency (or Laplacian, respectively) PST, PGST, or FR. If G admits PST with respect either to A or L, then we say that G admits PST. If G admits PST between vertices j and k, then we say that $\{j,k\}$ is a PST vertex pair, or that j and k pair up to have PST.

From Remark 1.3.2 we know that for any real symmetric matrix M, all of whose off-diagonal entries are non-negative or non-positive, there is an associated system with positive interaction strength (with positive edge weights) which has M as its Hamiltonian under certain dynamics (we are mainly considering the case of positive interaction strength, although negative strength seems realizable in practice and our results apply to this case too). The PST, PGST or FR properties of some systems can be seen to be closely related.

Proposition 1.3.9. *(i) For any given* $a \in \mathbb{R}$*, the system with Hamiltonian* $\mathcal{H} = M$ *exhibits PST if and only if the system with Hamiltonian* $M + aI$ *exhibits PST.*

(ii) For any given $a \in \mathbb{R}$*, the system with Hamiltonian* $\mathcal{H} = M$ *exhibits PST if and only if the system with Hamiltonian* $aI - M$ *admits PST.*

Proof. Since M and aI commute, $e^{it(M+aI)} = e^{ita}e^{itM}$, which implies part (i).

For a matrix $B = [b_{j,k}]$, denote by $\bar{B}$ the matrix $\left[\,\overline{b_{j,k}}\,\right]_{1\le j,k\le n}$. Part (ii) follows from the equalities $e^{it(aI-M)} = e^{ita}e^{-itM} = e^{ita}(e^{itM})^* = e^{ita}\overline{e^{itM}}$. $\square$

For a d-regular weighted or unweighted graph G on n vertices, from the fact that $L(G) = dI_n - A(G)$, we know that at any time t, for any two vertices j and k, the fidelity of state transfer between j and k with respect with $L(G)$ is the same as the fidelity of state transfer between j and k with respect to $A(G)$. This implies the following.

Proposition 1.3.10. *Let j and k be vertices of a* regular *weighted or unweighted graph. Then there is Laplacian PST, PGST, or FR between j and k if and only if there is adjacency PST, PGST, or FR between the two vertices.*

Proposition 1.3.9 shows that an overall energy shift on the Hamiltonian (from $\mathcal{H}$ to $\mathcal{H} + aI$) does not affect the occurrence or non-occurrence of PST, PGST or FR. The following remark shows that the same is true for scaling.

Remark 1.3.11. For any nonzero real number a, the system with Hamiltonian $\mathcal{H} = M$ exhibits PST, PGST or FR at time t_0 if and only if the system with Hamiltonian $\tilde{\mathcal{H}} = aM$ exhibits PST, PGST or FR at time $\frac{t_0}{a}$, since $e^{it_0(M)} = e^{i\frac{t_0}{a}(aM)}$ for any time $t_0 > 0$.

We want to transfer information fast. Consider the motivating example of transferring a quantum state within a quantum computer; for the computer to function efficiently, the state transfer would need to occur in a matter of nanoseconds. The above remark tells us that one way to achieve this is to scale the Hamiltonian by a big real number. However, the off-diagonal entries of M correspond to interaction strengths between quantum spins, which have an upper bound in order to be realizable in the real design. Therefore we do not consider the idea of achieving PST at a faster time by scaling the Hamiltonian, but this technique is important in the analysis.

1.4 Brief literature review

The early research of quantum state transfer was focused on (unweighted) graphs. Bose [17] first proposed the use of paths to transfer quantum states for short distance communication in a physical quantum computing schema. For graphs on n vertices, the path is a natural graph to consider, and it has the biggest diameter among all connected graphs with a given number of vertices, which means that in physical applications two spins at the endpoints are the furthest from each other. Christandl, Datta, Ekert and Landahl [31] found that unweighted paths on n vertices admit adjacency PST only for $n \leq 3$, and Laplacian PST only for $n \leq 2$.

To achieve high fidelity of quantum state transfer, we can consider paths that admit pretty good state transfer or other types of graphs that allow for perfect state transfer. For pretty good state transfer on paths, a complete characterization of the parameters (length of the unweighted path) for which there is adjacency PGST between the two end vertices of the path was given by Godsil, Kirkland, Severini and Smith [47], who showed that PGST occurs on an unweighted path with n vertices if and only if $n+1$ is either a prime number, two times a prime number, or a power of two. Later, a complete characterization of pretty good state transfer on paths between any pair of vertices was given by van Bommel [84]: pretty good state transfer occurs between vertices j and k on the unweighted path on n

vertices if and only if $(a)\, j + k = n + 1$, $(b)\, n + 1$ has at most one odd non-trivial divisor, and (c) if $n = 2^m r - 1$, for r odd and $r \neq 1$, then j is a multiple of 2^{m-1}.

There are many other families of graphs that admit perfect state transfer. Some examples are: a family of double-cone non-periodic graphs, certain joins of regular graphs with K_2 or with O_2 (see Angels-Canul, Norton, Opperman, Paribello, Russell and Tamon [4, 5]). Also, necessary and sufficient conditions for circulant graphs (Cayley graphs on the group $\mathbb{Z}_n$) to exhibit PST have been given by Bašić [11], and Bašić, Petković, and Stevanović [13]. The Cartesian product of two graphs both with PST at time t has also been shown to exhibit PST at time t (Godsil [45], Alvir, Dever, Lovitz, Myer, Tamon, Xu, and Zhan [2]); in particular the n-fold Cartesian product of K_2 with itself (the n-cube) has PST between its antipodal vertices. For a more general family of graphs — cubelike graphs — Bernasconi, Godsil and Severini [15] showed that if the sum of all the elements in the connection set is not $\mathbf{0}$, then there is PST in that graph at time $t = \frac{\pi}{2}$, and when the sum is $\mathbf{0}$, a necessary and sufficient condition for such a graph to admit PST is given by Cheung and Godsil [29]. However, a path is arguably the simplest graph structure, and since the graphs would need to be realized physically within a quantum computer, it is desirable to proceed with paths when possible, in order to minimize the amount of physical and technological resources required, so quantum state transfer on weighted paths (with or without loops) comes into the picture (we use the term "path" to mean an unweighted path).

Christandl, Datta, Dorlas, Ekert, Kay and Landahl [30] showed that for the adjacency matrix case, PST between the two end vertices of weighted paths (with vertices labelled $1, \ldots, n$) can be achieved over arbitrarily long distances (arbitrary n) by allowing for different edge weights; the weights used there to achieve adjacency PST are $w_{j,j+1} = \sqrt{j(n-j)}$ for each $j \in \{1, \ldots, n-1\}$. Another such set for even n is obtained by use of continued fractions and specially chosen eigenvalues [87]; using dual Hann polynomials, an edge weights set for a weighted path with loops on n vertices that admits adjacency PST between the end vertices is realized [1]. The case of other weights remains open. Vinet and Zhedanov [86] gave an eigenvalue characterization when a weighted path exhibits PST between its end vertices at a given time. Another way of making use of paths is to add weighted loops (called *potentials* in physics) on the vertices of an unweighted path, and it was believed that paths of arbitrary length n can be made to have PST between the end vertices by the addition of a set of suitable weighted loops [24, 73, 74]. Very recently (in 2017), Kempton, Lippner and Yau [64] showed that for paths on $n > 3$ vertices, any addition of weighted loops on the vertex set of the path does not help with achieving adjacency PST between the two end vertices. In the PGST setting, the same authors [64] showed that for any given graph with a pair of cospectral vertices, with a simple modification of the graph, along with a suitable addition of weighted loops on the vertex set, PGST can be achieved between the two cospectral vertices; in particular, the addition of a set of suitable weighted loops on the two end vertices of a path on n vertices yields PGST between the two end vertices.

As mentioned earlier, to achieve PST, the graph (system) has to be set up according to the parameters (set of fixed edge weights) in reality, and the state needs to be read out at a particular time. But even with lab equipment calibrated to an arbitrary amount of precision, the readout time might be $t + 0.0001$ instead of t for example, and some edge weight might be $w - 0.0001$ instead of w. We do not want the fidelity to drop drastically due to such errors. Bounds on the fidelity for such slightly perturbed systems are needed. In [59], Kay discusses the very issue of tolerance of a path with respect to timing errors and with respect to edge weight errors (so-called *manufacturing* errors). For timing errors, he derives a simple lower bound based on the squared difference between each eigenvalue and the smallest eigenvalue, noting that a Hamiltonian with minimal eigenvalue spread (the distance between the largest eigenvalue and smallest eigenvalue) would optimize the bound for small perturbations in readout time. For manufacturing errors, Kay finds that distances between eigenvalues are key, although no bound is given [59]. This sensitivity analysis was continued by Kirkland [66] through an analysis of the derivatives of the fidelity of state transfer with respect to either readout time or the weight $w_{j,k}$ of a fixed edge $\{j, k\}$. Under the hypothesis of perfect state transfer at time t_0 between vertices u and v, closed form expressions for $\frac{d^k p_{u,v}(t)}{dt^k}$ at t_0 for any $k \in \mathbb{N}$ were given. Those expressions then yield an easily computed lower bound on $p(t_0+h)$ for any small h. Again it was noted that minimizing the eigenvalue spread optimizes the bound on the fidelity of state transfer for small perturbations in time. Also expressions for the first two partial derivatives, $\frac{\partial p_{u,v}(t_0)}{\partial w_{j,k}}$ and $\frac{\partial^2 p_{u,v}(t_0)}{\partial^2 w_{j,k}}$, of $p_{u,v}(t)$ with respect to the edge weight $w_{j,k}$ under the hypothesis of perfect state transfer between u and v at t_0, were produced.

1.5 Structure of this thesis

In Chapter 2, we provide some graph theory and matrix theory background for this work. In Chapter 3, we consider a special class of graphs — graphs whose Laplacian matrix is diagonalizable by a Hadamard matrix, and obtain a simple spectral characterization for when such a graph has Laplacian perfect state transfer at time $\frac{\pi}{2}$ (since such graphs are regular, we know there is also adjacency PST at the same time). By using irrational weights in the "merge" graph operation (defined in Chapter 3), we produce graphs that have PGST from one vertex to three different vertices. We also prove that the n-cubelike graphs are exactly the family of (unweighted) graphs that are diagonalizable by the standard Hadamard matrix of order 2^n. Furthermore, we study uniform mixing on cubelike graphs and give a characterization of a particular family of cubelike graphs that admit uniform mixing at time $\frac{\pi}{4}$. In Chapter 4, we study perfect state transfer on weighted paths with respect to the Laplacian matrix, and perfect state transfer on weighted paths with (weighted) loops with respect to the adjacency matrix, by the use of orthogonal polynomials. The main result is that a weighted path on $n \geq 3$ vertices does not admit Laplacian PST between its end vertices at any time, nor does a special class of weighted symmetric trees between pairs of mirror-symmetric vertices. For the adjacency PST on a weighted path with or without loops, a rationality conjecture on the edge weights is given. In Chapter 5, we perform Godsil-McKay switching on the hypercube to create a new class of graphs that maintain many of the same properties as the hypercube. In particular, these graphs exhibit adjacency (and Laplacian) perfect state transfer between certain pairs of vertices. When PST occurs, the sensitivity of fidelity of state transfer with respect to timing errors is given. In Chapter 6, we analyze the sensitivity of the fidelity of state transfer, when adjacency PST or Laplacian PST occurs, with respect to small errors in readout time and in edge weights, and obtain some bounds on the fidelity. In Chapter 7, we consider a different, related, phenomenon — fractional revival — and we find that if there is Laplacian fractional revival between two vertices j and k, then the two vertices are strongly cospectral with respect to the Laplacian matrix L. We also give a complete characterization of threshold graphs that admit Laplacian fractional revival between a subset of two or more vertices. In Chapter 8, some problems for future study are listed.

Chapter 2

Background

2.1 Some matrix theory results

Recall that a square matrix A is said to be *symmetric* if $A^T = A$, *skew-symmetric* if $A^T = -A$, and *orthogonal* if $A^T A = I$. A complex square matrix A is said to be *Hermitian* if $A^* = A$, *skew-Hermitian* if $A^* = -A$, *unitary* if $A^* A = I$, and *normal* if $A^* A = AA^*$ [56].

2.1.1 Spectral decomposition of a Hermitian matrix

Eigenvalues and eigenvectors play important roles in the analysis of quantum information transfer. The multiset of all the eigenvalues (counting their multiplicities) of a matrix $B \in M_n$ is called the *spectrum* of B, denoted by $\sigma(B)$. Two non-isomorphic graphs are said to be *cospectral* with respect to the adjacency matrix (resp. Laplacian matrix) if the corresponding matrices of the two graphs have the same spectrum. An important nonnegative number associated to B, called the *spectral radius* of B, denoted by $\rho(B)$, is defined as the largest modulus among all the eigenvalues of B, that is, $\rho(B) = \max\{|\lambda| : \lambda \in \sigma(B)\}$. The spectra of some well-structured graphs are well-known. For example, the adjacency matrix of the complete graph K_n has only two distinct eigenvalues: $n-1$ with multiplicity 1, and -1 with multiplicity $n-1$. The Laplacian matrix of K_n also has exactly two distinct eigenvalues: 0 (simple) and n with multiplicity $n-1$. For arbitrary graphs, there are no direct formulas for all the eigenvalues. The following theorem tells us some information about where the eigenvalues are located.

Theorem 2.1.1. [56, Chapter 6]*(Gershgorin Theorem) Let $B = [b_{j,k}] \in M_n$, let*

$$R'_j(B) = \sum_{k \neq j} |b_{j,k}|, j = 1, \dots, n$$

denote the deleted row sums of B. The eigenvalues of B are in the union of Gershgorin discs

$$G(B) = \cup_{j=1}^{n} \{z \in \mathbb{C} : |z - b_{j,j}| \leq R'_j(B)\}.$$

Furthermore, if the union of ℓ of the n discs that comprise $G(B)$ forms a set $G_\ell(B)$ that is disjoint from the remaining $n - \ell$ discs, then $G_\ell(B)$ contains exactly ℓ eigenvalues of B, counted according to their algebraic multiplicities.

For a multiple eigenvalue λ of a diagonalizable matrix B, a list of orthonormal eigenvectors that form a basis of the eigenspace associated to the eigenvalue λ is not unique, but the orthogonal projection matrix onto each eigenspace is unique. For Hermitian matrices, we can say more.

Theorem 2.1.2. [44, Chapter 2]*(Spectral Decomposition) Let M be an $n \times n$ Hermitian matrix. Assume $\lambda_1, \ldots, \lambda_s$ are all the distinct eigenvalues of M, and for $j = 1, \ldots, s$, let E_j represent the orthogonal projection matrix onto the eigenspace associated with eigenvalue λ_j. Then the spectral decomposition of M is $M = \sum_{j=1}^{s} \lambda_j E_j$. Furthermore, the following hold:*

1. *$E_j^2 = E_j$ and $E_j E_k = 0$ if $j \neq k$.*

2. *$\sum_{j=1}^{s} E_j = I_n$.*

3. *If $f(x)$ is an analytic function which is defined at each eigenvalue of M, then $f(M) = \sum_{j=1}^{s} f(\lambda_j) E_j$.*

In particular, the adjacency matrix and the Laplacian matrix of a real-weighted or unweighted graph are real and symmetric, and therefore they have corresponding spectral decompositions. Assume G is a weighted or unweighted graph; denote its adjacency matrix by $A(G)$ and Laplacian matrix by $L(G)$. Let M be either $A(G)$ or $L(G)$. Assume the spectral decomposition of M is $M = \sum_{j=1}^{s} \lambda_j E_j$. Let k and ℓ be two vertices of G. If $(E_j)_{k,k} = (E_j)_{\ell,\ell}$ for each $j = 1, \ldots, s$, then we say k and ℓ are *cospectral* with respect to M, and if $E_j e_k = \pm E_j e_\ell$ for each j, then we say k and ℓ are strongly cospectral with respect to M. Since E_j is a symmetric idempotent, we know that $(E_j)_{k,k} = e_k^T E_j e_k = e_k^T E_j E_j e_k = e_k^T E_j^T E_j e_k = (E_j e_k)^T (E_j e_k)$, and hence strong cospectrality implies cospectrality of two vertices. Recall that for an invertible matrix B, $B^{-1} = \frac{1}{\det(B)} adj(B)$, where $adj(B)$ is the adjugate matrix of B. Combining this with Theorem 2.1.2 (3) for $f(x) = \frac{1}{\lambda - x}$, we have $\frac{\psi(G\backslash k,\lambda)}{\psi(G,\lambda)} = ((\lambda I - M)^{-1})_{k,k} = \sum_j \frac{(E_j)_{k,k}}{\lambda - \lambda_j}$, where $\psi(G,\lambda) = \det(\lambda I - M)$ is the characteristic polynomial of M, and $\psi(G\backslash k, \lambda)$ is the characteristic polynomial of the submatrix of M obtained from M by deleting the k-th row and k-th column. Therefore the definition of cospectral vertices is equivalent to the one given in Section 1.3.

Remark 2.1.3. [46] Making use of the spectral decomposition, we have $e^{itM} = \sum_{j=1}^{s} e^{it\lambda_j} E_j$, which plays a vital role in the analysis of quantum state transfer. For example, $A(K_2) = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ has $E_1 = \frac{1}{2}\begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$ associated to the eigenvalue $\lambda_1 = -1$, and $E_2 = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ associated to the eigenvalue $\lambda_2 = 1$. Therefore $e^{itA(K_2)} = \frac{1}{2}\begin{bmatrix} e^{it} + e^{-it} & e^{it} - e^{-it} \\ e^{it} - e^{-it} & e^{it} + e^{-it} \end{bmatrix} = \begin{bmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{bmatrix}$.

2.1.2 Matrix norms and some perturbation theory

Recall that for any vector $x \in \mathbb{C}^n$, its *Euclidean norm* $\|x\|_2$ is defined as $\|x\|_2 = \sqrt{x^* x}$. Now we introduce the definition of matrix norm and two specific matrix norms.

Definition 2.1.4. [56, Chapter 5] *A function* $|||\cdot||| : M_n \to \mathbb{R}$ *is a* matrix norm *if, for all* $A, B \in M_n$*, and any* $c \in \mathbb{C}$*, it satisfies the following five axioms:*

(1) $|||A||| \geq 0$ *Nonnegative*

(1a) $|||A||| = 0$ *if and only if* $A = 0$ *Positive*

(2) $|||cA||| = |c|\,|||A|||$ *Homogeneous*

(3) $|||A + B||| \leq |||A||| + |||B|||$ *Triangle inequality*

(4) $|||AB||| \leq |||A||| |||B|||$ *Submultiplicative*

The Frobenius norm $\|A\|_F$ and the spectral norm $|||A|||_2$ of a square matrix A are two commonly used matrix norms, both of which play important roles in the analysis of sensitivity of fidelity of state transfer with respect to edge weights.

Definition 2.1.5. [56, Chapter 5] *For a matrix $A = [a_{j,k}]$ of size $n \times m$, its* Frobenius norm *(also called the Schur norm) $\|A\|_F$ is defined as*

$$\|A\|_F = \sqrt{|\mathrm{Tr}(AA^*)|} = \sqrt{\sum_{j=1}^{n} \sum_{k=1}^{m} |a_{j,k}|^2},$$

where $\mathrm{Tr}(B)$ denotes the trace of a square matrix B, and $|a|$ denotes the modulus of the complex number a.

The spectral norm $|||A|||_2$ *of A is defined as*

$$|||A|||_2 = \sigma_1(A), \text{ the largest singular value of } A,$$

where the singular values of A are the square roots of all the (non-negative) eigenvalues of AA^*.

For a normal matrix A (that is, $AA^* = A^*A$), the singular values of A are the moduli of the eigenvalues of A, and therefore $|||A|||_2 = \rho(A)$ in this case [56, Chapter 5].

Definition 2.1.6. [56, Chapter 5] *A matrix norm $|||\cdot|||$ on M_n (resp. a vector norm $\|\cdot\|$ on $\mathbb{C}^n$) is said to be* unitarily invariant *if for any $A \in M_n$ (resp. any $x \in \mathbb{C}^n$) and any unitary matrix U of size n, $|||UA||| = |||A||| = |||AU|||$ (resp. $\|Ux\| = \|x\|$) holds.*

From the above definitions we can see that the Frobenius norm is unitarily invariant (this can be proved by using the fact that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$ for any matrices A, B such that the products are defined) and the spectral norm is unitarily invariant (this can be proved by using the fact that similar matrices have the same spectrum). Also the Euclidean vector norm $\|\cdot\|_2$ is unitarily invariant.

We also recall some important inequalities between the two matrix norms, the Euclidean norm of vectors, and the maximum modulus of matrix entries.

Theorem 2.1.7. [51, Section 2.3.2] *Let A be a real $m \times n$ matrix of rank r. Then*

$$\max_{j,k} |a_{j,k}| \leq |||A|||_2 \leq \|A\|_F \leq \sqrt{r}|||A|||_2,$$

$$|||A|||_2 \leq \sqrt{mn} \max_{j,k} |a_{j,k}|,$$

$$|||A|||_2 = \max_{\|x\|_2=1} \|Ax\|_2, \text{ and so } \|Ax\|_2 \leq |||A|||_2 \|x\|_2 \text{ for any } x \in \mathbb{C}^n \text{ and } A \in M_n.$$

The matrix exponential plays an important role throughout this thesis. The following Theorem shows that the power series $e^A = \sum_{k=0}^{\infty} \frac{1}{k!} A^k$ is well defined for every square matrix A.

Theorem 2.1.8. [56, Chapter 5] *Let A be any matrix of size $n \times n$, and let R be the radius of convergence of a scalar power series $\sum_{k=0}^{\infty} a_k z^k$. The matrix power series $\sum_{k=0}^{\infty} a_k A^k$ converges if the spectral radius of A satisfies $\rho(A) < R$. This condition is satisfied if there is a matrix norm $|||\cdot|||$ on M_n such that $|||A||| < R$.*

For example, $A(K_2)$ satisfies $(A(K_2))^{2k+1} = A(K_2)$ and $(A(K_2))^{2k} = I_2$, therefore $e^{itA(K_2)} = \sum_{j=0}^{\infty} \frac{i^j}{j!} (A(K_2))^j t^j = \sum_{j \text{ even}} \frac{(i)^j}{j!} t^j I_2 + \sum_{j \text{ odd}} \frac{(i)^j}{j!} t^j A(K_2) = \begin{bmatrix} \cos t & i \sin t \\ i \sin t & \cos t \end{bmatrix}.$

Sometimes we also make use of the inverse function of the exponential function — a logarithmic function. Given a matrix B, another matrix A is said to be a matrix logarithm of B if $e^A = B$. It is known that a matrix has a logarithm if and only if it is invertible [55]. In general, a logarithm of a matrix is not unique. The following theorem gives a formula to compute a (real) logarithm of a matrix that is sufficiently close to the identity matrix.

Theorem 2.1.9. [54, Section 2.3] *The function*

$$log(B) = \sum_{k=1}^{\infty} (-1)^{k+1} \frac{(B-I)^k}{k} = -\sum_{k=1}^{\infty} \frac{(I-B)^k}{k}$$

is defined and continuous on the set of all $n \times n$ complex matrices B with $\|B - I\|_F < 1$. For all B with $\|B - I\|_F < 1$, $e^{log(B)} = B$ holds.

When a matrix A is perturbed, a matrix function of A may also be perturbed. There is an important inequality telling us how sensitive the matrix exponential e^A is to perturbations in A when A is a normal matrix, in terms of the spectral matrix norm.

Theorem 2.1.10. [51, Chapter 9.3.2] *Let A be a normal matrix, E be a matrix of the same size as A, and t be a positive real number. Then*

$$\frac{\left|\!\left|\!\left| e^{(A+E)t} - e^{At} \right|\!\right|\!\right|_2}{|\!|\!| e^{At} |\!|\!|_2} \leq t |\!|\!| E |\!|\!|_2 e^{t |\!|\!| E |\!|\!|_2}.$$

It is known that all the eigenvalues of a Hermitian matrix are real numbers, so we can put them in order: let A be a Hermitian matrix, and order its eigenvalues in non-decreasing order as $\lambda_1(A) \leq \lambda_2(A) \leq \cdots \leq \lambda_n(A)$. We would like to know how the eigenvalues are influenced if A is perturbed by a Hermitian matrix. In the special case of a rank-one

Hermitian perturbation of a Hermitian matrix, the following *interlacing* theorem says that there is an easy rule to order the eigenvalues of the two matrices together without knowing the eigenvalues.

Theorem 2.1.11. [56, Chapter 4] *Let $n \geq 2$, let $A \in M_n$ be Hermitian, and let $z \in \mathbb{C}^n$ be nonzero. Then*

$$\lambda_1(A) \leq \lambda_1(A + zz^*) \leq \lambda_2(A) \leq \lambda_2(A + zz^*) \leq \cdots \leq \lambda_n(A) \leq \lambda_n(A + zz^*).$$

This theorem does not tell us directly how big $|\lambda_j(A + zz^*) - \lambda_j(A)|$ can be. The following bound on the corresponding eigenvalues of two general Hermitian matrices shows that it is bounded above by z^*z, as for any $z \in \mathbb{C}$, $|||zz^*|||_2 = z^*z$.

Theorem 2.1.12. [16, page 101] *Assume A and B are two Hermitian matrices of size n. Let $Eig^{\downarrow}(A)$ (resp. $Eig^{\downarrow}(B)$) denote a diagonal matrix whose diagonal entries are eigenvalues of A (resp. B) in non-increasing order. Then*

$$\left|\left|\left| Eig^{\downarrow}(A) - Eig^{\downarrow}(B) \right|\right|\right|_2 \leq |||A - B|||_2.$$

Sometimes we are also interested in the sensitivity of eigenvectors of a normal matrix to small perturbations. Assume M is a Hermitian matrix and λ is an eigenvalue of M with multiplicity r. It is known that there exists a set of r linearly independent eigenvectors of M associated to λ that depend continuously on entries of M. To be more specific, we have the following theorem.

Theorem 2.1.13. [3, 12] *Let $\delta \in \mathbb{R}$, $M(\delta)$ be a Hermitian $n \times n$ matrix with all its entries being analytic functions of the parameter δ in some open interval $\mathcal{I}_0$ that contains*

δ_0, that is, $M(\delta)$ can be seen as a function from $\mathbb{R}$ to M_n satisfying certain conditions. Assume that $\lambda_1(\delta_0)$ is an eigenvalue of $M(\delta_0)$ of multiplicity r. Then there exist r analytic functions $\lambda_1, \ldots, \lambda_r$: $\mathbb{R} \to \mathbb{C}$ and r linearly independent analytic vector-valued functions $x_1, \ldots, x_r$: $\mathbb{R} \to \mathbb{C}^n$, such that $M(\delta)x_j(\delta) = \lambda_j(\delta)x_j(\delta)$ throughout some open interval $\mathcal{I} \subseteq \mathcal{I}_0$ such that $\delta_0 \in \mathcal{I}$ and that $\lambda_1(\delta_0) = \cdots = \lambda_r(\delta_0)$.

This theorem tells us that for a Hermitian matrix M, for each of its eigenspaces, we can find a set of linearly independent vectors in this space that depend continuously on the entries of M. For eigenvectors associated to distinct eigenvalues of M, we also have some results. The following are from Bhatia [16]. Given a normal matrix A and a subset S of $\mathbb{C}$, we use $P_A(S)$ to denote the orthogonal projection onto the subspace spanned by the eigenvectors of A corresponding to those eigenvalues that lie in S. If S_1 and S_2 are two disjoint sets, and if $E = P_A(S_1)$ and $F = P_A(S_2)$, then E and F are mutually orthogonal, that is, $EF = 0$ (the eigenvectors of a normal matrix associated to distinct eigenvalues are orthogonal to each other). If A and B are two normal matrices, and if $E = P_A(S_1)$ and $F = P_B(S_2)$, then one might expect that if B is close to A and S_1 and S_2 are far apart, then E is nearly orthogonal to F. This is made precise in the theorem below.

Theorem 2.1.14. [16, Section 7.3] *Let A, B be two normal matrices. Let S_1 and S_2 be two subsets of the complex plane that are separated by either an annulus of width δ or a strip of width δ (there is a set $D \subset \mathbb{C}$, which is an annulus or strip of width δ such that S_1 and S_2 belong to different connected components of $\mathbb{C}\backslash D$). Let $E = P_A(S_1)$, $F = P_B(S_2)$.*

Then for every unitarily invariant matrix norm,

$$|||EF||| \leq \frac{1}{\delta}|||E(A-B)F||| \leq \frac{1}{\delta}|||A-B|||.$$

Another way to perturb a matrix is to border it. For a given Hermitian matrix M, order its eigenvalues in non-decreasing order as $\lambda_1(M) \leq \lambda_2(M) \leq \cdots \leq \lambda_n(M)$. Then we have the following *Cauchy's interlacing theorem for a bordered Hermitian matrix*, sometimes called the separation theorem.

Theorem 2.1.15. [56, Chapter 4] *Let B be an $n \times n$ Hermitian matrix, let $y \in \mathbb{C}^n$ and $a \in \mathbb{R}$ be given. Let $A = \begin{bmatrix} B & y \\ y^* & a \end{bmatrix} \in M_{n+1}$. Then*

$$\lambda_1(A) \leq \lambda_1(B) \leq \lambda_2(A) \leq \cdots \leq \lambda_n(A) \leq \lambda_n(B) \leq \lambda_{n+1}(A).$$

2.1.3 Weighted matrix tree theorem

Using the Laplacian matrix of a graph, we can compute the number of spanning trees of the graph directly.

Theorem 2.1.16. *(Kirchhoff's matrix tree theorem* [65][49, Chapter 13]*) Let G be a connected graph on n vertices, denote its Laplacian matrix by L, and its number of spanning trees by $t(G)$.*

1. *If the eigenvalues of L are $\lambda_1 = 0, \lambda_2, \ldots, \lambda_n$ (not necessarily distinct), then*

$$t(G) = \frac{\lambda_2 \cdots \lambda_n}{n}.$$

2. *For $1 \leq j \leq n$, let L_j be the reduced Laplacian obtained from L by deleting the j-th row and j-th column. Then*

$$t(G) = detL_j.$$

Since we are also working on weighted graphs, the following general version of the theorem is of important use.

Theorem 2.1.17. *(Weighted Matrix-Tree Theorem* [39]*) Let G be a weighted graph, and let $\hat{L}$ be its (weighted) Laplacian matrix.*

1. *If the eigenvalues of $\hat{L}$ are $\hat{\lambda}_1 = 0, \hat{\lambda}_2, \ldots, \hat{\lambda}_n$ (not necessarily distinct), then*

$$\sum_{T \in \Gamma(G)} \prod_{\{i,j\} \in E(T)} w_{i,j} = \frac{\hat{\lambda}_2 \cdots \hat{\lambda}_n}{n},$$

where $\Gamma(G)$ is the set of all spanning trees of G and $w_{i,j}$ is the weight of the edge between vertices i and j in T.

2. *For $1 \leq j \leq n$, let $\hat{L}_j$ be the reduced Laplacian obtained from $\hat{L}$ by deleting the j-th row and j-th column. Then*

$$\sum_{T \in \Gamma(G)} \prod_{\{i,j\} \in E(T)} w_{i,j} = det\hat{L}_j.$$

2.1.4 Symmetric functions of eigenvalues and principal minors of a matrix

First, recall some definitions related to a matrix.

Definition 2.1.18. [56, Chapter 0] *Let $A \in M_n$. For subsets $\alpha, \beta \subset \{1, \dots, n\}$, we denote by $A_{[\alpha,\beta]}$ the submatrix of entries that lie in the rows of A indexed by α and the columns indexed by β. If $\alpha = \beta$, the submatrix $A_{[\alpha]} = A_{[\alpha,\alpha]}$ is a* principal submatrix *of A. The determinant of an $r \times r$ submatrix of A is called a* minor *(of size r) of A. If the $r \times r$ submatrix is a principal submatrix, then its determinant is a* principal minor *(of size r).*

Therefore, for a matrix $A \in M_n$, each of its diagonal entries is a minor of A, and the determinant of A is a minor of A (of size n). As we know, for a given matrix A of size $n \times n$, its trace is the sum of all its eigenvalues and its determinant is the product of all its eigenvalues. In fact, there are more relations between the symmetric functions of the eigenvalues of A and the principal minors of A.

Definition 2.1.19. [56, Chapter 1] *Let $A \in M_n$. The sum of all its principal minors of size k (there are $\binom{n}{k}$ of them) is denoted by $E_k(A)$.*

The k-th elementary symmetric function of n complex numbers $\lambda_1, \dots, \lambda_n$, $k \le n$, is

$$S_k(\lambda_1, \dots, \lambda_n) = \sum_{1 \le i_1 < \cdots < i_k \le n} \prod_{j=1}^{k} \lambda_{i_j}$$

Notice that the sum above has $\binom{n}{k}$ summands. If $A \in M_n$ and $\lambda_1, \dots, \lambda_n$ are its eigenvalues, we define $S_k(A) = S_k(\lambda_1, \dots, \lambda_n)$.

Theorem 2.1.20. [56, Chapter 1] *Let $A \in M_n$. Then $S_k(A) = E_k(A)$ for each $k = 1, \dots, n$.*

2.2 Some graph operations

Recall that in this thesis, we refer to an undirected unweighted graph as a graph, and an undirected weighted graph as a weighted graph. Let $G = (V, E)$ denote the graph with vertex set V and edge set E. Then the *complement* G^c of G is the graph that has the same vertex set as G, and two vertices of G^c are adjacent if and only if they are not adjacent in G.

Definition 2.2.1. *Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs with disjoint vertex sets. Then*

1. *The* union $G_1 \cup G_2$ *of G_1 and G_2 is the graph with vertex set $V_1 \cup V_2$ and edge set $E_1 \cup E_2$, i.e., $G_1 \cup G_2 = (V_1 \cup V_2, E_1 \cup E_2)$.*

2. *The* join $G_1 \vee G_2$ *of G_1 and G_2 is $G_1 \vee G_2 = (G_1^c \cup G_2^c)^c$, which is the graph obtained by first taking the union of G_1 with G_2, and then connecting every vertex of G_1 to every vertex of G_2.*

3. *The* Cartesian product $G_1 \Box G_2$ *of G_1 and G_2 is the graph with vertex set $V_1 \times V_2$, and two vertices (u_1, u_2) and (v_1, v_2) are adjacent to each other if and only if one of the following two is true,*

   (a) $u_1 = v_1$, and u_2 and v_2 are adjacent in the graph G_2, or

   (b) $u_2 = v_2$, and u_1 and v_1 are adjacent in the graph 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 (u_1, u_2) and (u_1, v_2) in $G_1 \square G_2$ to be the same as the weight between u_2 and v_2 in G_2, and (ii) the weight of the edges between (u_1, u_2) and (v_1, u_2) in $G_1 \square G_2$ to be the same as the weight between u_1 and v_1 in G_1.

For example, the Cartesian product of the complete graph K_2 on two vertices with itself for n times gives us the n-cube (also called a hypercube). The adjacency matrix and the Laplacian matrix of the resulting graph with respect to each graph operation can be obtained from the corresponding matrices of the original graphs. Let G be a graph on n vertices with adjacency matrix $A(G)$ and Laplacian $L(G)$. Then $A(G^c) = J_{n,n} - I_n - A(G)$ and $L(G^c) = nI_n - J_{n,n} - L(G)$. Furthermore, the eigenvalues and eigenvectors of $L(G)$ and $L(G^c)$ are related as the following proposition shows.

Proposition 2.2.2. [49, Chapter 13] *Let G be a graph on $n \geq 2$ vertices. Assume that the eigenvalues of $L(G)$ are $0 = \lambda_1(G) \leq \lambda_2(G) \leq \cdots \leq \lambda_n(G)$, and that x_j is an eigenvector of $L(G)$ associated to the eigenvalue $\lambda_j(G)$. Denote the eigenvalues of $L(G^c)$ as $0 = \lambda_1(G^c) \leq \lambda_2(G^c) \leq \cdots \leq \lambda_n(G^c)$. Then for each $j = 2, \ldots, n$, $\lambda_j(G^c) = n - \lambda_{n+2-j}(G)$, and x_{n+2-j} is an eigenvector of $L(G^c)$ associated to the eigenvalue $\lambda_j(G^c)$.*

Before introducing the adjacency matrix for the Cartesian product of two graphs, we need to review another matrix operation — the tensor product.

Definition 2.2.3. *Let $A = [a_{j,k}]$ be an $m \times n$ matrix, and $B = [b_{r,s}]$ be a $p \times q$ matrix.*

Then the tensor product *of A with B is the $mp \times nq$ block matrix*

$$A \otimes B = \begin{bmatrix} a_{1,1}B & a_{1,2}B & \cdots & a_{1,n}B \\ a_{2,1}B & a_{2,2}B & \ddots & a_{2,n}B \\ \vdots & \vdots & \vdots & \vdots \\ a_{m,1}B & a_{m,2}B & \cdots & a_{m,n}B \end{bmatrix}.$$

Proposition 2.2.4. [57, Chapter 4] *The tensor product of matrices satisfies the following properties.*

1. *For any $m \times n$ matrix A, $p \times q$ matrix B, and any $\alpha \in \mathbb{C}$, $(\alpha A) \otimes B = A \otimes (\alpha B)$.*

2. *For any matrices A, B and C, $(A \otimes B) \otimes C = A \otimes (B \otimes C)$.*

3. *For any $p \times q$ matrix A, $r \times s$ matrix B, $q \times k$ matrix C, and $s \times \ell$ matrix D, $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$.*

Theorem 2.2.5. [36, Chapter 2; 40] *For $i = 1, 2$, let G_i be a graph on n_i vertices with adjacency matrix $A(G_i)$ and Laplacian matrix $L(G_i)$. Then the union $G_1 \cup G_2$ has adjacency matrix $A(G_1 \cup G_2) = \begin{bmatrix} A(G_1) & 0_{n_1,n_2} \\ 0_{n_2,n_1} & A(G_2) \end{bmatrix}$ and Laplacian matrix $L(G_1 \cup G_2) = \begin{bmatrix} L(G_1) & 0_{n_1,n_2} \\ 0_{n_2,n_1} & L(G_2) \end{bmatrix}$; the join $G_1 \vee G_2$ has adjacency matrix $A(G_1 \vee G_2) = \begin{bmatrix} A(G_1) & J_{n_1,n_2} \\ J_{n_2,n_1} & A(G_2) \end{bmatrix}$ and Laplacian matrix $L(G_1 \vee G_2) = \begin{bmatrix} L(G_1) + n_2 I_{n_1} & -J_{n_1,n_2} \\ -J_{n_2,n_1} & L(G_2) + n_1 I_{n_2} \end{bmatrix}$; the Cartesian product $G_1 \square G_2$ has adjacency matrix $A(G_1 \square G_2) = A(G_1) \otimes I_{n_2} + I_{n_1} \otimes A(G_2)$ and Laplacian matrix $L(G_1 \square G_2) = L(G_1) \otimes I_{n_2} + I_{n_1} \otimes L(G_2)$.*

The perfect state transfer property is closed under union as $e^{itA(G_1 \cup G_2)} = \begin{bmatrix} e^{itA(G_1)} & 0 \\ 0 & e^{itA(G_2)} \end{bmatrix}$; the following theorem shows that a similar result holds for Cartesian product. Note that the perfect state transfer property is not closed in general under the join operation.

Theorem 2.2.6. $[2, 45]$ *Let M denote the Laplacian matrix or adjacency matrix of a weighted or unweighted graph. Suppose G is a weighted or unweighted graph on m vertices and has perfect state transfer at time t between g_1 and g_2 with respect to M. Suppose Y is a weighted or unweighted graph on n vertices that has perfect state transfer at time t between y_1 and y_2 relative to M. Then $M(G \square Y) = M(G) \otimes I_n + I_m \otimes M(Y)$ implies that $e^{itM(G\square Y)} = e^{itM(G)} \otimes e^{itM(Y)}$. Therefore $G\square Y$ has perfect state transfer at time t between (g_1, y_1) and (g_2, y_2) relative to M.*

2.3 Partitions of a graph

2.3.1 Equitable partitions of a graph

Suppose that $G = (V, E)$ is a graph on n vertices, and let $A(G)$ denote the adjacency matrix of G. We review some properties of equitable partitions of $V(G)$ and the characteristic matrix P of the partition. Equitable partitions play an important role in the study of quantum state transfer with respect to the adjacency matrix.

Definition 2.3.1. [44, Chapter 5] *If $\pi = (C_1, \dots, C_k)$ is a partition of $V(G)$, the* characteristic matrix *P of π is the $n \times k$ matrix*

$$P_{j\ell} = \begin{cases} 1 & \text{if } v_j \in C_\ell, \\ 0 & \text{otherwise.} \end{cases}$$

If we scale each column of P so that its Euclidean norm is 1, then the resulting matrix is called the normalized characteristic matrix *of the partition π, and is denoted by $\hat{P}$.*

Note that $\hat{P}^T\hat{P} = I_k$.

Definition 2.3.2. [44, Chapter 5] *A partition $\pi = (C_1, \ldots, C_k)$ of $V(G)$ is* equitable *if for any $\ell, j \in \{1, \ldots, k\}$, the number of neighbours in C_ℓ of a vertex in C_j is the same for all vertices in C_j.*

For each graph with an equitable partition, we can associate a weighted directed graph to it, called the quotient graph, and a weighted undirected graph to it, called the symmetrized quotient graph.

Definition 2.3.3. [8, 44] *Given an equitable partition $\pi = (C_1, \ldots, C_k)$ of a graph $G = (V, E)$, let $c_{j\ell}$ denote the number of edges that join a fixed vertex in C_j to vertices in C_ℓ. Define the* quotient *G/π of G with respect to π to be the directed integer-weighted graph that has the cells of π as its vertices, and with an arc of weight $c_{j\ell}$ going from C_j to C_ℓ for each $c_{j\ell} \neq 0$. Define the* symmetrized quotient *$\widehat{G/\pi}$ of G with respect to π to be the undirected weighted graph that has the cells of π as its vertices, and with an edge of weight $\sqrt{c_{j\ell}c_{\ell j}}$ between C_j and C_ℓ for each $c_{j\ell} \neq 0$.*

Denote the adjacency matrix of the quotient graph G/π as $A(G/\pi)$ and the adjacency matrix of the symmetrized quotient graph $\widehat{G/\pi}$ by $A(\widehat{G/\pi})$. Then $A(G/\pi)_{j,\ell} = c_{j\ell}$, and $A(\widehat{G/\pi})_{j,\ell} = A(\widehat{G/\pi})_{\ell,j} = \sqrt{c_{j\ell}c_{\ell j}}$. An equitable partition can be characterized by the relation between the adjacency matrix of the graph and the normalized characteristic matrix $\hat{P}$ of the partition.

Proposition 2.3.4. [44, Chapter 5] *Let π be a partition of the vertex set of a graph G, with* *characteristic matrix P. If π is equitable then $A(G)P = PA(G/\pi)$. Conversely, if there is a matrix B such that $A(G)P = PB$, then π is an equitable partition and $B = A(G/\pi)$.*

Furthermore, an equitable partition can be characterized by the fact that A commutes with the matrix $\hat{P}\hat{P}^T$, where $\hat{P}$ is the normalized characteristic matrix of the partition.

Proposition 2.3.5. [46; 49, Chapter 9] *Suppose that $\pi = (C_1, \ldots, C_k)$ is a partition of the vertex set of a graph G, and that $\hat{P}$ is its normalized characteristic matrix. Then the following are equivalent:*

(a) π is equitable.

(b) The column space of $\hat{P}$ is $A(G)$-invariant.

(c) There is a matrix B of size $k \times k$ such that $A(G)\hat{P} = \hat{P}B$.

(d) A and $\hat{P}\hat{P}^T$ commute.

In the context of quantum state transfer with respect to the adjacency matrix of a graph, there is a nice connection between a graph G that admits a special equitable partition π of its vertex set and its symmetrized quotient graph $\widehat{G/\pi}$ with respect to π.

Theorem 2.3.6. [8, 26] *Let $G = (V, E)$ be a graph with an equitable partition π where vertices u and v belong to singleton cells. Then, for any time t,*

$$(e^{itA(G)})_{u,v} = (e^{itA(\widehat{G/\pi})})_{\{u\},\{v\}}, \tag{2.1}$$

where $\{u\}$ represents the singleton cell of π that contains u. Therefore, G admits adjacency perfect state transfer (resp. fractional revival) from u to v at time t if and only if the *symmetrized quotient graph $\widehat{G/\pi}$ admits adjacency perfect state transfer (resp. fractional revival) from $\{u\}$ to $\{v\}$ at time t; G admits adjacency PGST between u and v if and only if $\widehat{G/\pi}$ admits adjacency PGST from $\{u\}$ to $\{v\}$.*

2.3.2 Godsil-McKay switching

If we have an equitable partition π of a graph G, we can obtain a related symmetrized quotient graph $\widehat{G/\pi}$, which is usually a weighted graph. There is another type of partition of the vertex set of a graph, which is closely related to an equitable partition and can be used to produce a new unweighted graph that is cospectral to the original graph.

Theorem 2.3.7 (Godsil–McKay [48])**.** *Let G be a graph and let $\pi = (C_1, C_2, \cdots, C_k, D)$ be a partition of the vertex set $V(G)$. Suppose that, whenever $1 \leq i, j \leq k$ and $v \in D$, we have:*

(a) any two vertices in C_i have the same number of neighbours in C_j, and

(b) v has either 0, $n_i/2$ or n_i neighbours in C_i, where $n_i = |C_i|$.

(Note that π restricted on $G\backslash D$ is an equitable partition.) The graph $G^{(\pi)}$ formed by local switching in G with respect to π is obtained from G as follows: for each $v \in D$ and $1 \leq i \leq k$ such that v has $n_i/2$ neighbours in C_i, delete the corresponding $n_i/2$ edges and join v instead to the other $n_i/2$ vertices in C_i. Then $G^{(\pi)}$ and G are cospectral: for any positive integer r, if we define $\bar{Q}_r = 2J_r/r - I_r$, then the block diagonal matrix $Q = \operatorname{diag}(\bar{Q}_{n_1}, \bar{Q}_{n_2}, \ldots, \bar{Q}_{n_k}, I_{|D|})$ satisfies $Q^2 = I$, and $QA(G)Q = A(G^{(\pi)})$.

2.4 Hadamard matrices and Hadamard diagonalizable graphs

A *Hadamard matrix* of order n is an $n \times n$ matrix H with entries $+1$ and -1, such that $HH^T = nI$. Therefore, the inverse of a Hadamard matrix H of order n is $H^{-1} = \frac{1}{n}H^T$. It is known [53] that if there is a Hadamard matrix of order $n > 2$, then $4|n$.

Since the equality $(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$ holds for any matrices A, B, C and D such that the operations are defined, we know that the tensor product of two Hadamard matrices is still a Hadamard matrix. In particular, we can define a sequence of Hadamard matrices recursively; let

$$H_1 = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, H_2 = \begin{bmatrix} H_1 & H_1 \\ H_1 & -H_1 \end{bmatrix} = H_1 \otimes H_1, \ldots, H_n = \begin{bmatrix} H_{n-1} & H_{n-1} \\ H_{n-1} & -H_{n-1} \end{bmatrix} = H_1 \otimes H_{n-1}.$$

This construction gives the *standard* Hadamard matrix H_n of order 2^n.

From the definition of a Hadamard matrix, we know a $(1, -1)$ matrix is a Hadamard matrix if and only if any two rows of H are orthogonal, which is true if and only if any two columns of H are orthogonal. This mutual orthogonality 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 1s. A Hadamard matrix in this form is said to be *normalized* [85, page 199].

Given a graph G on n vertices with corresponding Laplacian matrix $L(G)$, if we can write $L(G) = \frac{1}{n}H\Lambda H^T$ for some Hadamard matrix H and some diagonal matrix Λ, then we say that G (or, that $L(G)$) is *Hadamard diagonalizable*. Hadamard diagonalizable graphs have some nice properties.

Theorem 2.4.1. [10, Theorem 5] *Let G be a graph on n vertices that is Hadamard diagonalizable. Then G is regular and all its Laplacian eigenvalues are even integers.*

A slightly stronger result is proved in Section 3.2 (Theorem 3.2.1). The following result allows us to make use of a more structured Hadamard matrix, namely, a normalized Hadamard matrix.

Lemma 2.4.2. [10, Lemma 4] *A graph G is Hadamard diagonalizable if and only if there is a normalized Hadamard matrix that diagonalizes $L(G)$.*

Thus, there is no loss of generality in assuming that the Laplacian matrix of 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 $|||H||| = 1$ for some matrix norm.

Being diagonalizable by a Hadamard matrix is preserved by many graph operations that we know.

Lemma 2.4.3 (Lemma 7, 8, [10])**.** *Let G be a Hadamard diagonalizable graph. Then G^c, $G \cup G$, and $G \vee G$ are also Hadamard diagonalizable. If Y is another Hadamard diagonalizable graph, then $G \square Y$ is also Hadamard diagonalizable. In fact, if G is diagonalizable by a Hadamard matrix $\hat{H}$ and Y is diagonalizable by a Hadamard matrix $\tilde{H}$, then G^c is* *diagonalizable by $\hat{H}$, $G \cup G$ and $G \vee G$ are diagonalizable by* $\begin{bmatrix} \hat{H} & \hat{H} \\ \hat{H} & -\hat{H} \end{bmatrix}$*, and $G \square Y$ is diagonalizable by $\hat{H} \otimes \tilde{H}$.*

Note that $G \vee Y$ is not necessarily Hadamard diagonalizable even if both G and Y are. For example, K_4 and C_4 (a cycle on 4 vertices) are both Hadamard diagonalizable, but $K_4 \vee C_4$ is not regular, and therefore not Hadamard diagonalizable by Theorem 2.4.1.

2.5 Cubelike graphs

2.5.1 The n-cube

Let K_2 denote the complete graph on 2 vertices, which is also called the 1-cube. For any integer $n \geq 1$, *the n-cube Q_n* (also called a *hypercube*) can be generated with the following two constructions.

The first construction is to define the graph by giving the vertex set and edge set of the graph: assigning a vertex to each of the 2^n binary strings of length n, connecting two vertices with an edge if and only if their binary labels differ at exactly one digit.

An equivalent way to define this graph is to use a graph operation, namely, the Cartesian product (Section 2.2). Taking the Cartesian product of K_2 with itself n times, denoted by $K_2^{\square n}$, also gives the n-cube. The n-cube is n-regular: each vertex has exactly n adjacent vertices.Direct computation (through the spectral decomposition, Theorem 2.1.2 and Remark 2.1.3, or through the power series formula of matrix exponential, the paragraph after Theorem 2.1.8) shows that K_2 admits perfect state transfer at time $\frac{\pi}{2}$:

$e^{itA(K_2)} = \begin{bmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{bmatrix}$. From Theorem 2.2.6 we know that, for any positive integer $n \geq 1$, the n-cube exhibits perfect state transfer at time $\frac{\pi}{2}$ between any pair of antipodal vertices (u and $u + \mathbf{1}$, where $\mathbf{1}$ is the all-ones vector, and the sum is performed in $\mathbb{Z}_2^n$).

Remark 2.5.1. Consider the first construction of Q_n. Let $V_1 = \{x \in \mathbb{Z}_2^n | wt(x) \equiv 0 \pmod 2\}$ and $V_2 = \{x \in \mathbb{Z}_2^n | wt(x) \equiv 1 \pmod 2\}$, where $wt(x)$ denotes the number of nonzero digits of x. Then every edge of Q_n has an end in V_1 and one end in V_2, which shows that Q_n is a bipartite graph. Now order the vertices of Q_n according to the bi-partition $V(Q_n) = V_1 \cup V_2$. Then the adjacency matrix is of the form $A(Q_n) = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}$ for some $2^{n-1} \times 2^{n-1}$ matrix B. From [32], we know that the unitary matrix $U_{Q_n}(t) = e^{itA(Q_n)}$ can be written as $U_{Q_n}(t) = \begin{bmatrix} M_1(t) & iK(t) \\ iK^T(t) & M_2(t) \end{bmatrix}$ for some real matrices $M_1(t), M_2(t)$ and $K(t)$.

2.5.2 Cayley graphs and cubelike graphs

Hypercubes are highly symmetric structures; in fact, they are vertex-transitive. There is a more general family of graphs that are vertex-transitive: the Cayley graphs, whose definition is based on a group.

Definition 2.5.2. [49, Chapter 3] *Let $\mathcal{G}$ be a group and let C be a subset of $\mathcal{G}$ that is closed under taking inverses and does not contain the identity. Then the* Cayley graph $G = \mathcal{G}(C)$ *is the graph with vertex set $\mathcal{G}$ and edge set $\{\{u, v\} : uv^{-1} \in C\}$, and C is called the connection set of G.*

Recall that a subset S of a group $\mathcal{G}$ is a generating set for $\mathcal{G}$ if every element of $\mathcal{G}$ can be written as a product of elements of S. The connectedness of the Cayley graph $G = \mathcal{G}(C)$ can be determined from its connection set C.

Theorem 2.5.3. [49, Chapter 3] *The Cayley graph $G = \mathcal{G}(C)$ is connected if and only if C is a generating set for $\mathcal{G}$.*

The n-cube is a Cayley graph for the abelian group $\mathbb{Z}_2^n$, with connection set $C = \{e_1, \ldots, e_n\}$. More generally, any Cayley graph for $\mathbb{Z}_2^n$ is called an *n-cubelike graph*. From the definition we know the Cayley graph $G = \mathcal{G}(C)$ is a $|C|$-regular graph. Furthermore, as we will see in Corollary 3.6.2 [15], a graph is diagonalizable by a standard Hadamard matrix if and only if it is a cubelike graph. The following result characterizes PST of cubelike graphs at time $\pi/2$, where the summation is performed in the abelian group $\mathbb{Z}_2^n$ and $\mathbf{0}$ is the zero vector in $\mathbb{Z}_2^n$.

Theorem 2.5.4. [15, Theorem 1], [29, Theorem 2.3] *Let C be a subset of $\mathbb{Z}_2^n$ and let σ be the sum of the elements of C. If $\sigma \neq \mathbf{0}$, then PST occurs in $\mathbb{Z}_2^n(C)$ from j to $j + \sigma$ at time $\pi/2$. If $\sigma = \mathbf{0}$, then $\mathbb{Z}_2^n(C)$ is* periodic *with period $\pi/2$ (that is, $\mathbb{Z}_2^n(C)$ is periodic at all its vertices at time $\pi/2$).*

2.6 Perfect state transfer

2.6.1 Perfect state transfer and rows of the diagonalization matrix

First recall the Cauchy-Schwarz inequality, which plays an important role in the study of perfect state transfer.

Theorem 2.6.1. *For any two vectors $u, v \in \mathbb{C}^n$, the following inequality holds*

$$|u \cdot v|^2 \leq \|u\|_2 \cdot \|v\|_2,$$

where $\| \cdot \|_2$ denote the Euclidean norm of a vector, and the inner product $u \cdot v$ is $u^* v$. Furthermore, equality holds if and only if u and v are linearly dependent.

If G admits PST, then the rows of a real orthogonal matrix Q that diagonalizes the Hamiltonian $\mathcal{H}$ need to satisfy some conditions.

Proposition 2.6.2. [60] *Suppose that G is a a weighted or unweighted graph with Hamiltonian $\mathcal{H}$ and that $Q^T \mathcal{H} Q = \Lambda$, where $Q = [q_{j,k}]_{1 \leq j,k \leq n}$ is real orthogonal and Λ is diagonal. Denote the ℓ-th row of Q as q_ℓ^T. Then G admits PST between vertices j and k at time t_0 if and only if $e^{it_0\Lambda} q_k = e^{i\phi} q_j$ (or equivalently, $q_k^T e^{it_0\Lambda} = q_j^T e^{i\phi}$) for some $\phi \in \mathbb{R}$.*

Proof. A weighted graph G with Hamiltonian $\mathcal{H}$ admits PST at time $t_0 > 0$ between two vertices j and k if and only if $p_{j,k}(t_0) = |e_j^T e^{it_0\mathcal{H}} e_k|^2 = 1$. As shown in equations (1.2) and (1.3), we know that

$$p_{j,k}(t_0) = |q_j^T e^{it_0\Lambda} q_k|^2 \tag{2.2}$$

Since $\|q_j\|_2 = 1$ and $\|e^{it_0\Lambda}q_k\|_2 = 1$, Cauchy-Schwarz inequality implies that the value in equation (2.2) is equal to 1 if and only if $e^{it_0\Lambda}q_k = e^{i\phi}q_j$ for some $\phi \in \mathbb{R}$. □

In summary, if G admits perfect state transfer between vertices j and k, and Q is a real orthogonal matrix that diagonalizes the Hamiltonian $\mathcal{H}$ of G, then the corresponding entries in the j-th row and k-th row of Q have the same modulus (in fact they are equal, or one is the negative of the other, since Q is a real matrix). Furthermore, we need the eigenvalues and the readout time t_0 to work together to adjust the signs of the entries ($e^{it_0\Lambda}q_k = e^{i\phi}q_j$).

2.6.2 A necessary condition on the weights for a weighted path to exhibit PST between the end vertices

Assume G is a weighted path with loops. A necessary and sufficient condition that the eigenvalues of the adjacency matrix $A(G)$ must satisfy for G to admit adjacency PST between its end vertices is shown in Section 4.1.3. The following is a necessary condition that the weights of edges and loops of G must satisfy for G to exhibit PST between its end vertices.

Lemma 2.6.3. [61] *If a weighted path with loops with Hamiltonian*

$$\mathcal{H} = \begin{bmatrix} b_1 & j_1 & 0 & \cdots & 0 & 0 \\ j_1 & b_2 & j_2 & \cdots & 0 & 0 \\ 0 & j_2 & b_3 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & b_{n-1} & j_{n-1} \\ 0 & 0 & 0 & \cdots & j_{n-1} & b_n \end{bmatrix}$$

admits perfect state transfer between its two end vertices, then the Hamiltonian $\mathcal{H}$ must satisfy $j_\ell^2 = j_{n-\ell}^2$ and $b_\ell = b_{n+1-\ell}$ for all ℓ. In particular, since we are considering positive weights, $j_\ell = j_{n-\ell}$.

2.6.3 Sensitivity of fidelity of state transfer to changes in time when PST occurs

Assume a weighted graph G admits PST between vertices u and v at time $t = t_0$. If the state is read out at vertex v at time $t_0 + h$ instead of t_0 due to some small errors h in time, what is the probability that the state read out is the same as the one sent from u (if the state is read out at time t_0, then the probability is 1), or how sensitive is the fidelity of transfer to changes in the readout time? To answer this question, the derivatives of the fidelity of state transfer with respect to the readout time have been analyzed [66]. When PST occurs, the following result provides expressions for the derivatives of the fidelity of transfer between vertices u and v of all orders in terms of the diagonal entries of powers of $\mathcal{H}$.

Theorem 2.6.4. [66] *Assume a weighted graph G with Hamiltonian $\mathcal{H}$ admits PST between vertices u and v at time $t = t_0$. Denote the fidelity of state transfer $p_{u,v}(t)$ between vertices u and v by p for short. For each $j \in \mathbb{N}$, let $w(j) = e_u^T \mathcal{H}^j e_u$, and set $w(0) = 1$. Then for each $k \in \mathbb{N}$,*

$$\frac{d^k p}{dt^k}\Big|_{t=t_0} = \begin{cases} (-1)^{(k \pmod 4)/2} \sum_{j=0}^{k} (-1)^j \binom{k}{j} w(j) w(k-j), & \textit{if } k \textit{ is even,} \\ 0 & \textit{if } k \textit{ is odd.} \end{cases} \tag{2.3}$$

In particular, if G is an unweighted graph, then $\frac{d^2p}{dt^2}|_{t=t_0} = -2\deg(u)$ if $\mathcal{H} = A(G)$, as $w(1) = 0$ and $w(2) = \deg(u)$ in this case, and $\frac{d^2p}{dt^2}|_{t=t_0} = -2\deg(u)$ if $\mathcal{H} = L(G)$, as $w(1) = \deg(u)$ and $w(2) = \deg(u)^2 + \deg(u)$ in this case.

2.6.4 More properties about perfect state transfer

For a given graph G, if there is PST from vertex j to vertex k at time t_0, then there is no PST from j to any other vertex $\ell(\neq k)$ at time t_0 (since each row of $e^{it\mathcal{H}}$ has norm 1, where $\mathcal{H}$ is the Hamiltonian of the graph). But is it possible for G to admit PST from vertex j to vertex k at time t_0, and PST from vertex j to vertex $\ell \neq j, k$ at a different time t_1? That is, it is possible that $p_{j,k}(t_1) = 1$ and $p_{j,\ell}(t_2) = 1$ for some three distinct vertices j, k and ℓ of the graph G? The following result tells us that the answer is no.

Proposition 2.6.5 ([60]). *If a graph admits perfect state transfer from j to k and from j to ℓ, then $k = \ell$.*

The proof of the theorem uses the minimum periodicity of a graph at a vertex and the minimum time for PST at this vertex. Here we give an independent proof without making use of periodicity.

Alternate proof of Proposition 2.6.5: Without loss of generality we can reindex the vertices in such a way that it suffices to show that if there is PST from vertex 1 to vertex 2 at time t_1, then it is impossible to have PST from vertex 1 to vertex 3 at time t_2. We proceed by contradiction. Let M denote the adjacency matrix or Laplacian matrix of the graph G on n vertices, and assume it is diagonalized by a real orthogonal matrix

$Q = [q_{j,k}]_{1 \le j,k \le n}$ to $\Lambda = \mathrm{diag}\,(\lambda_1, \cdots, \lambda_n)$, that is, $Q^T M Q = \Lambda$. Denote the j-th row of Q by q_j^T. Since there is PST from vertex 1 to vertex 2 at time t_1, by Proposition 2.6.2, we have that $e^{-it_1\Lambda} q_1 = e^{-i\theta} q_2$ for some $\theta \in \mathbb{R}$, which is equivalent to

$$q_1^T e^{it_1\Lambda} e^{-i\theta} = q_2^T. \tag{2.4}$$

Similarly, the assumption that there is PST from vertex 1 to vertex 3 at time t_2 implies that for some $\alpha \in \mathbb{R}$

$$q_1^T e^{it_2\Lambda} e^{-i\alpha} = q_3^T. \tag{2.5}$$

Thus $q_{1,j} = 0$ if and only if $q_{2,j} = 0$ (if and only if $q_{3,j} = 0$), and for each j such that $q_{1,j} \neq 0$, we have $e^{i(t_1\lambda_j - \theta)} = \pm 1$, $e^{i(t_2\lambda_j - \alpha)} = \pm 1$, since q_1, q_2 and q_3 are real vectors. Let S be the set of indices j (where $q_{1,j} \neq 0$) such that $e^{i(t_1\lambda_j - \theta)} = 1$ (that is $q_{1,j} = q_{2,j}$), and T be the set of indices j such that $e^{i(t_1\lambda_j - \theta)} = -1$ (that is $q_{1,j} = -q_{2,j}$). Then from $\|q_1\| = 1$ and the fact that q_1 and q_2 are orthogonal to each other, it follows that $\sum_{j\in S} q_{1,j}^2 + \sum_{j\in T} q_{1,j}^2 = 1$ and $\sum_{j\in S} q_{1,j}^2 - \sum_{j\in T} q_{1,j}^2 = 0$, and therefore $\sum_{j\in S} q_{1,j}^2 = \sum_{j\in T} q_{1,j}^2 = 1/2$ with $S \neq \emptyset$ and $T \neq \emptyset$. Now we show there is some $\ell \in S$ such that $e^{i(t_2\lambda_\ell - \alpha)} = 1$. If not, the equation $\sum_{j\in S} q_{1,j} q_{3,j} = -\sum_{j\in S} q_{1,j}^2 = -1/2$, combined with the fact that q_1 and q_3 are orthogonal, would yield $\sum_{j\in T} q_{1,j} q_{3,j} = 1/2$. Since $\sum_{j\in T} q_{1,j}^2 = 1/2$, and $q_{3,j} = \pm q_{1,j}$ for $j \in T$, it follows that $q_{3,j} = q_{1,j}$ for all $j \in T$, thus $q_3 = -q_2$, contradicting the fact that Q is real orthogonal matrix. So for some $\ell \in S$, $e^{i(t_1\lambda_\ell - \theta)} = e^{i(t_2\lambda_\ell - \alpha)} = 1$; that is, $e^{i\theta} = e^{it_1\lambda_\ell}$ and $e^{i\alpha} = e^{it_2\lambda_\ell}$. Substituting these into equations (2.4) and (2.5), we have

$$q_1^T e^{it_1\Lambda} e^{-it_1\lambda_\ell} = q_2^T, \quad q_1^T e^{it_2\Lambda} e^{-it_2\lambda_\ell} = q_3^T. \tag{2.6}$$

For each $j \in S \cup T \equiv W$, we have $t_1(\lambda_j - \lambda_\ell) = k_j\pi$, and $t_2(\lambda_j - \lambda_\ell) = k'_j\pi$ for some integers $k_j,\ k'_j$. For $\lambda_j = \lambda_\ell$, we have $j \in S$, k_j and k'_j are both even, and $q_{1,j} = q_{2,j} = q_{3,j}$. For $\lambda_j \neq \lambda_\ell$, in particular for $j \in T \neq \emptyset$, since the left sides of the two equations (below equation (2.6)) are not zero, neither are the right sides. Therefore we have $\frac{k_j}{k'_j} = \frac{k_j\pi}{k'_j\pi} = \frac{t_1(\lambda_j - \lambda_\ell)}{t_2(\lambda_j - \lambda_\ell)} = \frac{t_1}{t_2}$, which is a fixed number (independent of j). Since k_j and k'_j are integers, the above result is a rational number, say r/s for some relatively prime integers r and s. Therefore $k'_j = k_j s/r$. Since k'_j is an integer, $r|k_j s$, and since r and s are relatively prime, we have $r|k_j$. Note that for $j \in S$, k_j is an even integer, and for $j \in T$, k_j is an odd integer. Since T is not empty, we know r is an odd integer. If s is even, then k'_j is even for all $j \in W$, which combined with equation (2.6) implies $q_{1,j}e^{it_2\lambda_j}e^{-it_2\lambda_\ell} = q_{1,j}e^{ik'_j\pi} = q_{3,j}$ for $j \in W$, and therefore $q_1 = q_3$, a contradiction. Thus s is odd, but this implies that k_j and k'_j have the same parity for each $j \in W$. Again from equation (2.6), we obtain $q_2 = q_3$, which is impossible in a real orthogonal matrix. Therefore there is no PST from one vertex to several different vertices. $\square$

Chapter 3

Perfect quantum state transfer using Hadamard diagonalizable graphs

In this chapter, we focus on quantum state transfer under Laplacian dynamics, and on a specific class of graphs — graphs whose Laplacian matrix can be diagonalized by a Hadamard matrix. As mentioned in Proposition 2.6.2, if there is PST between vertices j and k of graph G, then for a real orthogonal matrix Q which diagonalizes $L(G)$, the corresponding entries in its j-row and k-th row are either equal to or are the negative of each other. Hadamard diagonalizable matrices certainly satisfy this condition for any pair of vertices, and we just need to make sure that the eigenvalues and readout time work nicely with the sign between the corresponding entries in the two rows. As we will see in Theorem 3.2.1, weighted or unweighted Hadamard diagonalizable graphs are regular, so the results we get here about Laplacian PST (PGST) also hold for adjacency

PST (PGST), as mentioned in Remark 1.3.10. Furthermore, integer-weighted graphs with Hadamard diagonalizable Laplacian matrix are convenient to work with in our setting because their spectra consist entirely of even integers (Theorem 3.2.1); consequently the corresponding graph often exhibits PST between two of its vertices at time $t_0 = \pi/2$ (see Theorem 3.2.2 for a more specific statement). This chapter is based on work with Johnston, Kirkland, Plosker and Storey [58]. The work began when Johnston visited the University of Manitoba in May 2016 for a one-week period. Storey was Plosker's undergraduate student research assistant in Summer 2016.

3.1 Introduction

Let n be a positive integer. Complete graphs K_{4n} are known to be Hadamard diagonalizable (provided that there is a Hadamard matrix of that order) [10], but such graphs do not admit perfect state transfer [18]. There is another family of graphs that are known to be Hadamard diagonalizable [15]: the cubelike graphs, which have highly symmetric structure and have been relatively well-studied. Complete characterizations of perfect state transfer properties of cubelike graphs are given [15, 29]. In this chapter, we will see that cubelike graphs are closely related to standard Hadamard matrices. Hadamard diagonalizablity is closed under many graph operations such as complement, union, join, and Cartesian product as mentioned in Lemma 2.4.3. Here we construct another binary operation on weighted graphs — the merge operation — under which Hadamard diagonalizability is also kept. There is a graph operation closely related to our merge operation — the "$\ltimes$" operation; perfect state transfer with respect to this operation is studied in [33].

Let $G_1 = (V_1, E_1)$ and $G_2 = (V_2, E_2)$ be two graphs. If $V_1 = V_2$, then $G_1 \ltimes G_2$ is the graph with adjacency matrix $A(G_1 \ltimes G_2) = \begin{bmatrix} A(G_1) & A(G_2) \\ A(G_2) & A(G_1) \end{bmatrix}$. 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 $A(G_1) + A(G_2)$.

In this chapter, an eigenvalue characterization of weighted Hadamard diagonalizable graphs that admit PST at time $t = \frac{\pi}{2}$ is given. By Remark 1.3.11, we know that if all the (integer) weights of an integer-weighted Hadamard diagonalizable graph have a nontrivial common factor, the characterization can be used to study the PST property of such graphs at other times as well.

The structure of this chapter is as follows. In Section 3.2, we give a simple eigenvalue characterization for when a weighted Hadamard diagonalizable graph admits perfect state transfer at time $\pi/2$; this characterization allows one to choose correct eigenvalues to build (weighted, might also have negative weights) Hadamard diagonalizable graphs having perfect state transfer (Example 3.2.3). In Section 3.3, we observe that Hadamard diagonalizable graphs that admit PST at time $\frac{\pi}{2}$ are not that rare, in the sense that there are connected unweighted non-bipartite d-regular such graphs on 2^k vertices for each positive integer d satisfying $k + 1 \leq d \leq 2^k - 2$. Also we show that the existence of PST is maintained under graph complementation and the join operation, if we restrict to the class of

Hadamard diagonalizable graphs that have PST at time $\frac{\pi}{2}$. In Section 3.4, we introduce the "merge" operation, a weighted variant of the "$\ltimes$" operation, which takes two graphs with the same number of vertices as input, and produces a new (larger) graph. In particular, the merge of two graphs which are diagonalizable by the same Hadamard matrix is still Hadamard diagonalizable. We also characterize when the merge of two integer-weighted graphs that are diagonalizable by the same normalized Hadamard matrix exhibits PST. In Section 3.5, we give some results concerning the optimality in terms of timing errors and manufacturing (edge weight) errors of Hadamard diagonalizable graphs. We also give an optimality result, showing that among regular graphs of degree $r \leq 4$, the r-cube is the sparsest Hadamard diagonalizable connected unweighted graph with perfect state transfer at time $\pi/2$. In Section 3.6, we characterize the family of graphs that are diagonalizable by the standard Hadamard matrix H_n of size 2^n for any positive integer n, showing a direct relationship to cubelike graphs. Further, we study uniform mixing on cubelike graphs, and for the cubelike graphs that are obtained from the hypercube by adding one or two more elements in the connection set, we give a characterization of the one or two added elements when the resulting cubelike graph admits uniform mixing at time $\frac{\pi}{4}$.

3.2 Eigenvalue characterization of Hadamard diagonalizable graphs with PST at time $\frac{\pi}{2}$

The following theorem originally appeared in [10], restricted to the case of unweighted graphs. The version below allows for arbitrary integer edge weights. Although the proof is almost identical to the unweighted version, we include it here for completeness.

Theorem 3.2.1. [10, Theorem 5] *If G is a weighted or unweighted graph that is Hadamard diagonalizable, then G is regular; if in addition G is integer-weighted, then all its Laplacian eigenvalues are even integers.*

Proof. Without loss of generality we assume that G is a weighted or unweighted graph on n vertices and that the Laplacian matrix $L(G)$ is diagonalized by a normalized Hadamard matrix H (Lemma 2.4.2) to a diagonal matrix $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$.

First we show that G is regular. Fix an index $j \in \{1, \dots, n\}$, and let S_j be the diagonal matrix with diagonal entries ± 1 such that $e_j^T H S_j = \mathbf{1}^T$. Observe that HS_j is also a Hadamard matrix, and that $H^{-1}L(G)H = \Lambda$, or equivalently, $L(G)H = H\Lambda$ implies that $L(G)HS_j = H\Lambda S_j = HS_j\Lambda$. Since the j-th row of HS_j is the all-ones vector and the remaining rows are orthogonal to it, we deduce that $HS_j\mathbf{1} = ne_j$. Consequently, $ne_j^T L(G)e_j = e_j^T L(G)(HS_j\mathbf{1}) = e_j^T(L(G)HS_j)\mathbf{1} = e_j^T(HS_j\Lambda)\mathbf{1} = (e_j^T HS_j)\Lambda\mathbf{1} = \mathbf{1}^T\Lambda\mathbf{1}$. Thus, for each $j = 1, \dots, n$, $e_j^T L(G)e_j = \frac{1}{n}\mathbf{1}^T\Lambda\mathbf{1}$, so G is regular, as desired.

Now assume in addition that G is integer-weighted; observe that the first column of H is the all-ones vector, and that it is an eigenvector of $L(G)$ corresponding to the eigenvalue

0. For any non-zero eigenvalue λ_j of $L(G)$, the j-th column of H is an eigenvector associated to λ_j. One can split the graph G into two subgraphs, G_1 and G_2 (with Laplacians $L(G_1)$ and $L(G_2)$), corresponding to the $n/2$ entries of 1 and the $n/2$ entries of -1 of He_j. By applying a permutation similarity if necessary, we find that

$$\begin{bmatrix} L(G_1)+X_1 & -R \\ -R^T & L(G_2)+X_2 \end{bmatrix} \begin{bmatrix} \mathbf{1}_{\frac{n}{2}} \\ -\mathbf{1}_{\frac{n}{2}} \end{bmatrix} = \lambda_j \begin{bmatrix} \mathbf{1}_{\frac{n}{2}} \\ -\mathbf{1}_{\frac{n}{2}} \end{bmatrix},$$

for some matrices X_1, X_2, and R. Necessarily X_1, X_2 are diagonal, and note that $X_1\mathbf{1}_{\frac{n}{2}} = R\mathbf{1}_{\frac{n}{2}}$ and $X_2\mathbf{1}_{\frac{n}{2}} = R^T\mathbf{1}_{\frac{n}{2}}$.

Since $\lambda_j\mathbf{1}_{\frac{n}{2}} = L(G_1)\mathbf{1}_{\frac{n}{2}} + X_1\mathbf{1}_{\frac{n}{2}} + R\mathbf{1}_{\frac{n}{2}} = 2X_1\mathbf{1}_{\frac{n}{2}}$, and since G is integer-weighted (and therefore all the entries of X_1 are integers), we deduce that λ_j is an even integer. Hence each eigenvalue of the integer-weighted Laplacian matrix is an even integer.

□

We now give a precise characterization of the eigenvalues of a weighted Hadamard diagonalizable graph that exhibits PST at time $t_0 = \pi/2$. The proof applies a standard characterization of PST; see Proposition 2.6.2 or [60], for example. Recall that a graph is Hadamard diagonalizable if and only if it is diagonalizable by a normalized Hadamard matrix (Theorem 2.4.2).

Theorem 3.2.2. *Let G be a weighted Hadamard diagonalizable graph on n vertices. Let $H = [h_{u,v}]$ be a corresponding normalized Hadamard matrix. Denote the eigenvalues of the Laplacian matrix $L(G)$ by $\lambda_1, \cdots, \lambda_n$, so that $L(G)He_\ell = \lambda_\ell He_\ell$, $\ell = 1, \ldots, n$. Then G has PST from vertex j to vertex k at time $t_0 = \pi/2$ if and only if $\lambda_1, \ldots, \lambda_n$ are all even* *integers and for each* $\ell = 1, \cdots, n$, $\lambda_\ell \equiv 1 - h_{j,\ell} h_{k,\ell} \pmod 4$.

Proof. Let $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$, then $L(G) = \frac{1}{n} H \Lambda H^T$, and hence $e^{i(\pi/2)L(G)} = \frac{1}{n} H e^{i(\pi/2)\Lambda} H^T$. By Proposition 2.6.2, it follows that G admits 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 $\mathbf{1}$, i.e. an eigenvector of $L(G)$ corresponding to the eigenvalue 0, we know that the first entry of $e^{i(\pi/2)\Lambda} H^T e_j$ is $e^{i(\pi/2)0} h_{j,1} = h_{j,1} = 1$, and the first entry of $H^T e_k$ is $h_{k,1} = 1$. 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., G admits PST from vertex j to k at $\pi/2$ if and only if

$$e^{i(\pi/2)\Lambda} H^T e_j = H^T e_k. \tag{3.1}$$

Note that this implies that $\lambda_1 \ldots, \lambda_n$ are all even integers, and that

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

Consequently, equation (3.1) holds if and only if, for each $\ell = 1, \cdots, n$, if $h_{j,\ell} h_{k,\ell} = 1$ then $\lambda_\ell \equiv 0 \pmod 4$, and if $h_{j,\ell} h_{k,\ell} = -1$ then $\lambda_\ell \equiv 2 \pmod 4$. The conclusion follows. $\square$

It is worth noting that Theorem 3.2.2 gives an 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 for some two rows j and k of H, and then $L(G) = \frac{1}{n} H \Lambda H^T$ will necessarily be the Laplacian matrix of some rational-weighted graph (possibly with negative weights) with PST at time $t_0 = \pi/2$ (the graph will be integer-weighted provided n divides each entry of $H \Lambda H^T$).

Example 3.2.3. Now making use of Theorem 3.2.2, we construct weighted graphs on 4 vertices that admit PST at time $\pi/2$ between vertices 1 and 3 and that are diagonalizable by the normalized Hadamard matrix $H = H_2 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$. Note that $h_{1,1}h_{3,1} = h_{1,2}h_{3,2} = 1$ and $h_{1,3}h_{3,3} = h_{1,4}h_{3,4} = -1$. Now construct a diagonal matrix $\Lambda = \operatorname{diag}(0, \lambda_2, \lambda_3, \lambda_4)$ with $\lambda_\ell \equiv 1 - h_{1,\ell}h_{3,\ell} \pmod 4$ for $\ell = 2, 3, 4$. For example, let $\Lambda = \operatorname{diag}(0, 4, 2, 6)$. We know the weighted graph with Laplacian $L_1 = \frac{1}{4}H\Lambda H^T = \begin{bmatrix} 3 & -2 & -1 & 0 \\ -2 & 3 & 0 & -1 \\ -1 & 0 & 3 & -2 \\ 0 & -1 & -2 & 3 \end{bmatrix}$ is a required weighted graph by Theorem 3.2.2. Letting $\Lambda = \operatorname{diag}(0, 4, 2, 2)$, we obtain $L_2 = \frac{1}{4}H\Lambda H^T$; this is the Laplacian matrix of the 2-cube, which is known to exhibit PST at time $\pi/2$. Similarly, letting $\lambda_2 = 2 \equiv h_{1,2}h_{2,2} \pmod 4$, $\lambda_3 = 4 \equiv h_{1,3}h_{2,3} \pmod 4$, and $\lambda_4 = 6 \equiv h_{1,4}h_{2,4} \pmod 4$ yields the Laplacian matrix $L_3 = \frac{1}{4}H\Lambda H^T$ of a weighted Hadamard diagonalizable graph that admits PST between vertices 1 and 2 at time $\pi/2$.

3.3 Existence of Hadamard diagonalizable graphs with PST

The degree of a Hadamard diagonalizable graph with PST can have a wide range, in the sense that the corresponding graph can range from very sparse (few edges) to very dense (many edges).

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 the fact that the adjacency matrix of any cubelike graph (and hence the Laplacian matrix, since cubelike graphs are regular) is diagonalizable by the standard Hadamard matrix [15] and by using Theorem 2.5.4. To ensure that the cubelike graph is connected, we just need to make sure that its connection set contains a basis of $\mathbb{Z}_2^k$ when considered as a vector space. Let $T = \{e_1, \ldots, e_k\}$, where $e_1, \ldots, e_k$ form a standard basis for $\mathbb{Z}_2^k$. For $d = k+1$, take the connection set $C = T \cup \{e_1 + e_2\}$. Then the induced subgraph on vertices $\mathbf{0}, e_1, e_2$ and $e_1 + e_2$ is K_4; hence the corresponding cubelike graph is not bipartite. Also note that the sum of the elements in C is not $\mathbf{0}$ for $k \geq 3$. For $d > k+1$, select any S such that $C \subseteq S$, $|S| = d$ and $\mathbf{0} \notin S$. If the sum of all elements in S is not $\mathbf{0}$, then the cubelike graph $\mathbb{Z}_2^k(S)$ is a desired graph. On the other hand, if the sum of all elements in S is $\mathbf{0}$, then we replace some element c_0 from the set $S \setminus C$ by any element $c_1 \in \mathbb{Z}_2^k \setminus (S \cup \{\mathbf{0}\})$ (this set has cardinality $2^k - d - 1 > 0$) and form a new set $S_1 = (S \cup \{c_1\}) \setminus \{c_0\}$. Then S_1 has cardinality d and the sum of all its elements is $c = c_0 + c_1 \neq \mathbf{0}$. 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 $\mathbb{Z}_2^k$) non-bipartite cubelike graph $\mathbb{Z}_2^k(S_1)$.

This observation can be stated as follows.

Theorem 3.3.1. *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) admits PST between distinct vertices at time $t_0 = \pi/2$.

Example 3.3.2. Making use of the arguments at the beginning of this section, we can construct graphs satisfying properties (1), (2), and (3) of Theorem 3.3.1. Consider graphs on $2^3 = 8$ vertices, and let $e_1 = \begin{bmatrix}1\\0\\0\end{bmatrix}, e_2 = \begin{bmatrix}0\\1\\0\end{bmatrix}, e_3 = \begin{bmatrix}0\\0\\1\end{bmatrix}$. The cubelike graph $\mathbb{Z}_2^3(C_1)$ with $C_1 = \{e_1, e_2, e_3, e_1 + e_2\}$ is a connected 4-regular (4 elements in the connection set C_1) graph that is diagonalizable by the standard Hadamard matrix H_3 (as it is a cubelike graph) and admits PST at time $\frac{\pi}{2}$ (from Theorem 2.5.4 and the fact that the sum of the elements in the connection set C_1 is $e_3 \neq \mathbf{0}$). Similarly, the cubelike graph $\mathbb{Z}_2^3(C_2)$ with $C_2 = \{e_1, e_2, e_3, e_1 + e_2, e_2 + e_3\}$ is a required 5-regular graph, the cubelike graph $\mathbb{Z}_2^3(C_3)$ with $C_3 = \{e_1, e_2, e_3, e_1 + e_2, e_2 + e_3, e_1 + e_2\}$ is a required 6-regular graph, and the cubelike graph $\mathbb{Z}_2^3(C_4)$ with $C_4 = \{e_1, e_2, e_3, e_1 + e_2, e_2 + e_3, e_1 + e_2, e_1 + e_2 + e_3\}$ is a required 7-regular graph.

As mentioned in Section 2.2, we know that the union of a graph exhibiting PST with itself still exhibits PST, which is not true in general for the join operation. In the class of Hadamard diagonalizable graphs, there are more properties about PST with respect to these operations. 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 3.3.3. *Let G be a graph on $n \geq 4$ vertices that is diagonalizable by a*

Hadamard matrix H. If G admits perfect state transfer between vertex j to vertex k at time $t_0 = \pi/2$, then so does its complement G^c and the join $G \vee G$.

Proof. Without loss of generality we can assume that H is a normalized Hadamard matrix (by Lemma 2.4.2). If we denote the eigenvalues of the Laplacian matrix of G by $\lambda_1 = 0, \lambda_2, \cdots, \lambda_n$, then from Theorem 3.2.2 we know that for $\ell = 1, \cdots, n$, $\lambda_\ell \equiv 1 - h_{j,\ell}h_{k,\ell} \pmod 4$. From Lemma 2.4.3, we know that G^c, $G \cup G$, and $G \vee G$ are all Hadamard diagonalizable. Combined with Proposition 2.2.2, $L(G^c)$ is diagonalized by the same Hadamard matrix H to $\operatorname{diag}(0, n - \lambda_2, \cdots, n - \lambda_n)$. Since $1 - h_{j,\ell}h_{k,\ell}$ is either 0 or $2 \pmod 4$ and n must be a multiple of 4 in order for a Hadamard matrix of order $n \geq 4$ to exist, the eigenvalues $0, n - \lambda_2, \ldots, n - \lambda_n$ of G^c satisfy $(n - \lambda_\ell) \equiv -(1 - h_{j,\ell}h_{k,\ell}) \equiv 1 - h_{j,\ell}h_{k,\ell} \pmod 4$. Again from Theorem 3.2.2, we know that G^c has PST from vertex j to k at time $\pi/2$. The result that G^c admits PST between vertices j and k (and hence so does the union of G^c with itself) and that $G^c \cup G^c$ is Hadamard diagonalizable implies that $G \vee G = (G^c \cup G^c)^c$ also has PST from vertex j to k at time $\pi/2$. $\square$

3.4 Merge of two weighted graphs

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 $L(G_1) = D(G_1) - A(G_1)$ and $L(G_2) = D(G_2) - A(G_2)$, 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 weighted graph $G_1 \; {}_{w_1}\!\odot_{w_2} \, G_2$ with Laplacian

$$\begin{bmatrix} w_1 L(G_1) + w_2 D(G_2) & -w_2 A(G_2) \\ -w_2 A(G_2) & w_1 L(G_1) + w_2 D(G_2) \end{bmatrix}.$$

Note that the merge operation is defined for labelled graphs. Different labelling of G_1 or G_2 might produce non-isomorphic $G_1 \; {}_{w_1}\!\odot_{w_2} \, G_2$.

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

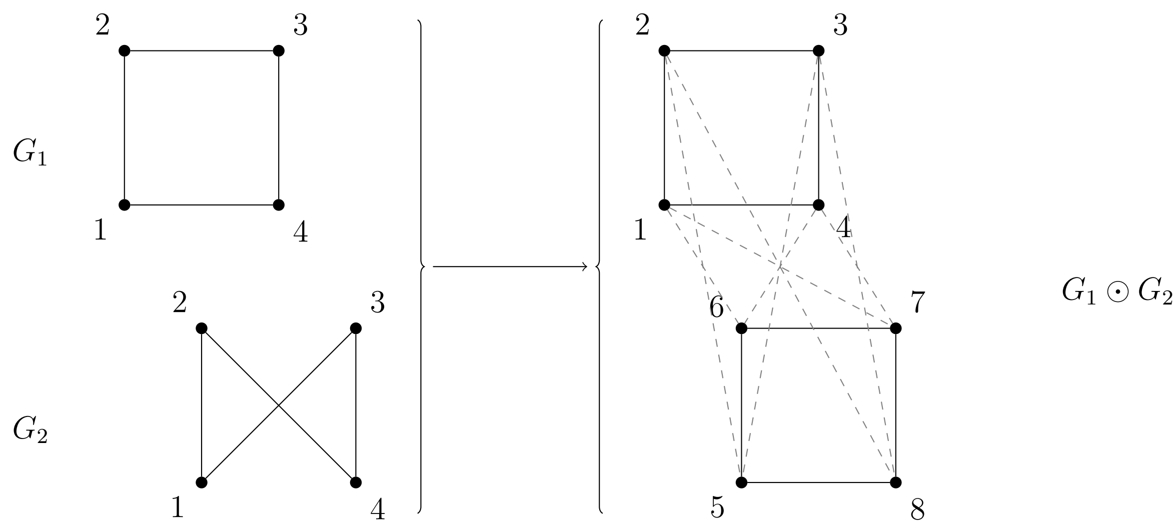


Figure 3.1: A depiction of two Hadamard diagonalizable graphs (left) with vertex set $\{1, \ldots, n\}$ and their merge (right). The merge $G_1 \odot G_2$ has vertex set $V(G_1) \cup V(G_2)$; for $j, k \le n$, there is an edge $\{j, k\}$ and $\{n + j, n + k\}$ in the new graph if and only if G_1 had edge $\{j, k\}$, and there is an edge $\{j, n + k\}$ in the new graph if and only if G_2 had edge $\{j, k\}$.

Our definition of the merge is motivated by the following fact.

Proposition 3.4.1. *If G_1 and G_2 are both diagonalizable by the same Hadamard matrix H, then $G_1 \; {}_{w_1}\!\odot_{w_2} \; G_2$ is also Hadamard diagonalizable, by the matrix* $\begin{bmatrix} H & H \\ H & -H \end{bmatrix}$.

While the merge is a bit less intuitive than the other graph operations 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 $w_{j,k}$ then $G_1 \; {}_{w_1}\!\odot_{w_2} \; G_2$ has edges $\{j, k\}$ and $\{n+j, n+k\}$, each with weight $w_1 w_{j,k}$. Similarly, if G_2 has edge $\{j, k\}$ with weight $w_{j,k}$ then $G_1 \; {}_{w_1}\!\odot_{w_2} \; G_2$ has edges $\{j, n+k\}$ and $\{k, n+j\}$ with weight $w_2 w_{j,k}$. See Fig. 3.1 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

$$L(G_1) = \begin{bmatrix} 2 & -1 & 0 & -1 \\ -1 & 2 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ -1 & 0 & -1 & 2 \end{bmatrix}, \quad L(G_2) = \begin{bmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}, \text{and}$$

$$L(G_1 \odot G_2) = \begin{bmatrix} 4 & -1 & 0 & -1 & 0 & -1 & -1 & 0 \\ -1 & 4 & -1 & 0 & -1 & 0 & 0 & -1 \\ 0 & -1 & 4 & -1 & -1 & 0 & 0 & -1 \\ -1 & 0 & -1 & 4 & 0 & -1 & -1 & 0 \\ 0 & -1 & -1 & 0 & 4 & -1 & 0 & -1 \\ -1 & 0 & 0 & -1 & -1 & 4 & -1 & 0 \\ -1 & 0 & 0 & -1 & 0 & -1 & 4 & -1 \\ 0 & -1 & -1 & 0 & -1 & 0 & -1 & 4 \end{bmatrix}.$$

3.4.1 PST property of the merge $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ when both w_1 and w_2 are integers

We now describe an exact characterization of when the merge of two integer-weighted graphs which are diagonalizable by the same normalized 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 graphs with perfect state transfer in a variety of scenarios. In the following proof, keep in mind that an integer-weighted Hadamard diagonalizable graph has only even integer eigenvalues, and therefore $(2k)\lambda \equiv 0 \pmod 4$ and $(2k+1)\lambda \equiv -(2k+1)\lambda \pmod 4$ for any eigenvalue λ and any integer k.

Theorem 3.4.2. *Suppose G_1 and G_2 are (labelled) integer-weighted graphs on n vertices, both of which are diagonalizable by the same normalized Hadamard matrix H. Fix $w_1, w_2 \in \mathbb{Z}$ and let $L(G_1) = d_1 I - A(G_1)$, $L(G_2) = d_2 I - A(G_2)$ be the Laplacian matrices of G_1, G_2, respectively (for $j = 1, 2$, d_j is the degree of G_j). Then for two integers w_1 and w_2, the integer-weighted graph $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ has PST from vertex j to k, where $j < k$, at time $t_0 = \pi/2$ if and only if one of the following 8 conditions holds:*

1. *$j, k \in \{1, \ldots, n\}$ and*

    (a) *w_1 is odd, w_2 is even, and G_1 has PST from j to k at $t_0 = \pi/2$, or*

    (b) *w_1 and d_2 are even, w_2 is odd, and G_2 has PST from j to k at $t_0 = \pi/2$, or*

    (c) *w_1 and w_2 are odd, d_2 is even, and the weighted graph with Laplacian $L(G_1)+L(G_2)$ has PST from j to k at $t_0 = \pi/2$;*

2. *$j, k \in \{n+1, \ldots, 2n\}$ and*

   (a) *w_1 is odd, w_2 is even, and G_1 has PST from $j-n$ to $k-n$ at $t_0 = \pi/2$, or*

   (b) *w_1 and d_2 are even, w_2 is odd, and G_2 has PST from $j-n$ to $k-n$ at $t_0 = \pi/2$, or*

   (c) *w_1 and w_2 are odd, d_2 is even, and the weighted graph with Laplacian $L(G_1) + L(G_2)$ has PST from $j-n$ to $k-n$ at $t_0 = \pi/2$;*

3. *$j \in \{1, \ldots, n\}$, $k \in \{n+1, \ldots, 2n\}$ and*

   (a) *w_1 is even, w_2 and d_2 are odd, and G_2 has PST from j to $k-n$ at $t_0 = \pi/2$, or*

   (b) *w_1, w_2, and d_2 are all odd, and the weighted graph with Laplacian matrix $L(G_1) + L(G_2)$ has PST from j to $k-n$ at $t_0 = \pi/2$.*

Proof. Denote the diagonal matrices of eigenvalues for $L(G_1), L(G_2)$ by Λ_1, Λ_2, respectively, so that $L(G_j) = \frac{1}{n} H \Lambda_j H^T$, $j = 1, 2$. Then the Laplacian of $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ is $L(G_1 \ {}_{w_1}\!\odot_{w_2} G_2) = \begin{bmatrix} w_1 L(G_1) + w_2 d_2 I & -w_2 A(G_2) \\ -w_2 A(G_2) & w_1 L(G_1) + w_2 d_2 I \end{bmatrix}$. Further,

$$L(G_1 \, {}_{w_1}\!\odot_{w_2} G_2) = \frac{1}{2n} \begin{bmatrix} H & H \\ H & -H \end{bmatrix} \begin{bmatrix} w_1 \Lambda_1 + w_2 \Lambda_2 & 0 \\ 0 & w_1 \Lambda_1 - w_2 \Lambda_2 + 2 w_2 d_2 I \end{bmatrix} \begin{bmatrix} H & H \\ H & -H \end{bmatrix}^T.$$

Denote the eigenvalues of $L(G_1), L(G_2)$ by $\lambda_\ell^{(1)}, \lambda_\ell^{(2)}$, $\ell = 1, \cdots, n$, respectively.

1. Suppose that $j, k \in \{1, \cdots, n\}$ and that the weighted graph $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ admits PST from vertex j to k at time $\pi/2$. Then by Theorem 3.2.2, for each $\ell = 1, \cdots, n$,

$$w_1 \lambda_\ell^{(1)} + w_2 \lambda_\ell^{(2)} \equiv (1 - h_{j,\ell} h_{k,\ell}) \pmod 4, \text{ and} \tag{3.2}$$

$$w_1\lambda_\ell^{(1)} - w_2\lambda_\ell^{(2)} + 2w_2d_2 \equiv (1 - h_{j,\ell}h_{k,\ell}) \pmod 4. \tag{3.3}$$

Summing the above two congruences gives $2w_1\lambda_\ell^{(1)}+2w_2d_2 \equiv 2w_2d_2 \equiv 0 \pmod 4$, where we used the fact that $\lambda_\ell^{(1)}$ is an even integer for each ℓ in the above congruence equality. Therefore w_2d_2 is even. Note that if w_1 and w_2 are both even, then (3.2) implies that $h_{j,\ell}h_{k,\ell} = 1$ for $\ell = 1, \cdots, n$, which is impossible.

If w_1 is odd and w_2 is even, then $w_1\lambda_\ell^{(1)}+w_2\lambda_\ell^{(2)} \equiv \lambda_\ell^{(1)} \pmod 4$, and equation (3.2) simplifies to $\lambda_\ell^{(1)} \equiv (1 - h_{j,\ell}h_{k,\ell}) \pmod 4$, $\ell = 1, \cdots, n$. Hence G_1 has PST from j to k by Theorem 3.2.2. Similarly, if w_1 is even and w_2 is odd, then necessarily d_2 is even, and as above it can be shown that G_2 has PST from j to k.

If w_1 and w_2 are both odd, then necessarily d_2 is even. In this case, equation (3.2) gives $w_1\lambda_\ell^{(1)} + w_2\lambda_\ell^{(2)} \equiv \lambda_\ell^{(1)} + \lambda_\ell^{(2)} \equiv (1 - h_{j,\ell}h_{k,\ell}) \pmod 4$, $\ell = 1, \cdots, n$. We deduce that the weighted graph with Laplacian $L(G_1) + L(G_2)$ has PST from j to k at time $t_0 = \pi/2$.

2. If $j, k \in \{n+1, \cdots, 2n\}$ and the weighted graph $G_1 \,{}_{w_1}\!\odot_{w_2} G_2$ has PST from j to k at time $t_0 = \pi/2$, then the conclusions (a), (b), and (c) follow analogously to Case 1 above.

3. Suppose that $j \in \{1, \cdots, n\}$, $k \in \{n+1, \cdots, 2n\}$ and that the weighted graph $G_1 \,{}_{w_1}\!\odot_{w_2} G_2$ has PST from j to k. Set $\hat{k} = k - n$. Then for each $\ell = 1, \cdots, n$,

$$w_1\lambda_\ell^{(1)} + w_2\lambda_\ell^{(2)} \equiv (1 - h_{j,\ell}h_{\hat{k},\ell}) \pmod 4, \text{ and} \tag{3.4}$$

$$w_1\lambda_\ell^{(1)} - w_2\lambda_\ell^{(2)} + 2w_2d_2 \equiv (1 + h_{j,\ell}h_{\hat{k},\ell}) \pmod 4. \tag{3.5}$$

Summing equations (3.4) and (3.5), we find that $2w_1\lambda_\ell^{(1)} + 2w_2d_2 \equiv 2 \pmod 4$ and hence $2w_2d_2 \equiv 2 \pmod 4$. 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 (3.4) simplifies to $\lambda_\ell^{(2)} \equiv (1 - h_{j,\ell}h_{\hat{k},\ell}) \pmod 4$, $\ell = 1, \cdots, n$, so if w_1 is even, and both w_2 and d_2 are odd, then G_2 has PST from j to $\hat{k}$.

If w_1 is odd, then (3.4) simplifies to $\lambda_\ell^{(1)} + \lambda_\ell^{(2)} \equiv (1 - h_{j,\ell}h_{\hat{k},\ell}) \pmod 4$, $\ell = 1, \cdots, n$, which shows that the integer-weighted graph with Laplacian $L(G_1) + L(G_2)$ has PST from j to $\hat{k}$.

The converses are straightforward. $\square$

Note that when both w_1 and w_2 are even, the graph $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ does not admit 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 $G_1 \ {}_{\frac{w_1}{2^r}}\!\odot_{\frac{w_2}{2^r}} G_2$, which has Laplacian $\frac{1}{2^r}L(G_1 \ {}_{w_1}\!\odot_{w_2} G_2)$, at time $\pi/2$ can be determined according to Theorem 3.4.2. In the case that PST occurs, the graph $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ would then have PST at time $\pi/2^{r+1}$.

Example 3.4.3. 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 normalized Hadamard matrix. Suppose that G_1 admits PST from vertex j to vertex k, 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 j to $k + 2^m$ according to Case 3(b) in

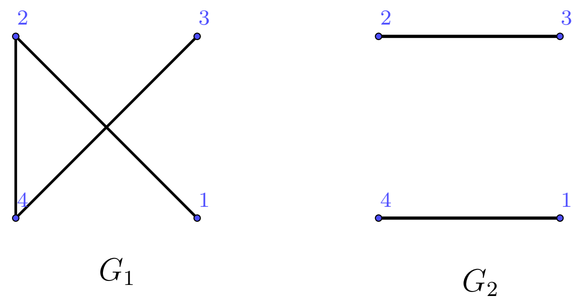


Figure 3.2: Without the condition that the two graphs are diagonalizable by the same normalized Hadamard matrix, Theorem 3.4.2 is not necessarily true

Theorem 3.4.2. Similarly, $G_2 \odot G_1$ has PST from vertex j to k if d_1 is even (Case 1(c)), and it has PST from vertex j to $k + 2^m$ if d_1 is odd (Case 3(b)).

Theorem 3.4.2 is not necessarily true without the condition that the two graphs are diagonalizable by the same normalized Hadamard matrix. Let G_1 and G_2 be two labelled graphs as shown in Figure 3.2. Then the graph $G_1 \odot G_2$ does not admit PST at time $\pi/2$, though the parameters are set up so that they satisfy 3(b) of Theorem 3.4.2 (but not the hypothesis of both Laplacians being diagonalizable by the same Hadamard: here G_2 is diagonalizable by the standard Hadamard matrix H_2, and G_1 is not Hadamard diagonalizable). Thus, unlike a similar result [33, Theorem 5.2] for the "$\ltimes$" operation (which uses the adjacency matrices), graphs whose Laplacian matrices are not 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.

Note that we require the two weighted graphs G_1 and G_2 in Theorem 3.4.2 to be integer-weighted to ensure that all of their Laplacian eigenvalues are even integers. By checking the proof it can be observed that the conclusion of the theorem still holds if G_1 and G_2 only have even integer eigenvalues, but are not necessarily integer-weighted.

Example 3.4.4. From Lemma 9 and Proposition 10 [10] we know that there are exactly 4 graphs on 12 vertices that are Hadamard diagonalizable: K_{12}, $O_{12} = K_{12}^c$, $K_6 \cup K_6$, and $K_{6,6} = (K_6 \cup K_6)^c$. By making use of the fact that the complete graph K_n on $n \geq 3$ vertices does not admit PST, one can conclude that K_{12} and $K_6 \cup K_6$ do not admit Laplacian/adjacency PST. Or more generally, using of the idea in the proof of Theorem 3.2.2, we know that a Hadamard diagonalizable graph admit PST at time t_0 if and only if $e^{it_0\Lambda}H^T e_j = H^T e_k$, where H is a normalized Hadamard matrix that diagonalizes $L(G)$ to Λ as in Thereom 3.2.2. But the eigenvalues of $L(K_{6,6})$ are 0 with multiplicity 1, 6 with multiplicity 10, and 12 with multiplicity 1. The above equality does not hold for any t_0. Hence $K_{6,6}$ does not admit Laplacian PST. Therefore no unweighted graph of order 12 that is Hadamard diagonalizable exhibits PST. However, it is possible to construct weighted graphs of this type. Let G_1 be the graph whose Laplacian is

$$L(G_1) = \frac{1}{3}\begin{bmatrix} 18 & 0 & -1 & -1 & -1 & -3 & -3 & -3 & -1 & -3 & -1 & -1 \\ 0 & 18 & -1 & -1 & -1 & -3 & -3 & -3 & -1 & -3 & -1 & -1 \\ -1 & -1 & 18 & -2 & -2 & 0 & -2 & 0 & -2 & -2 & -4 & -2 \\ -1 & -1 & -2 & 18 & -4 & 0 & 0 & -2 & -2 & -2 & -2 & -2 \\ -1 & -1 & -2 & -4 & 18 & -2 & -2 & 0 & -2 & 0 & -2 & -2 \\ -3 & -3 & 0 & 0 & -2 & 18 & -2 & -2 & 0 & -2 & -2 & -2 \\ -3 & -3 & -2 & 0 & -2 & -2 & 18 & -2 & -2 & -2 & 0 & 0 \\ -3 & -3 & 0 & -2 & 0 & -2 & -2 & 18 & -2 & -2 & -2 & 0 \\ -1 & -1 & -2 & -2 & -2 & 0 & -2 & -2 & 18 & 0 & -2 & -4 \\ -3 & -3 & -2 & -2 & 0 & -2 & -2 & -2 & 0 & 18 & 0 & -2 \\ -1 & -1 & -4 & -2 & -2 & -2 & 0 & -2 & -2 & 0 & 18 & -2 \\ -1 & -1 & -2 & -2 & -2 & -2 & 0 & 0 & -4 & -2 & -2 & 18 \end{bmatrix}.$$

Direct computation shows that $L(G_1)$ is Hadamard diagonalizable by the order 12 Hadamard matrix

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

All the eigenvalues of $L(G_1)$ are even integers (which are 0, 4, 8, 8, 8, 8, 6, 6, 6, 6, 6, 6), and that the $(1, 2)$ entry of $e^{i(\pi/2)L(G_1)}$ is 1, thus showing that G_1 exhibits PST between vertices 1 and 2 at time $t_0 = \pi/2$. Let $G_2 = K_{12}$, which is Hadamard diagonalizable by H but does not exhibit PST. As $L(G_1)$ and $L(G_2)$ only have even integer eigenvalues, Case 1(a) of the Theorem 3.4.2 tells us that the weighted graph $G_1 \; {}_5{\odot}_2 \; G_2$ admits PST from vertex 1 to vertex 2 at time $t_0 = \pi/2$.

3.4.2 Rational weights or when $\frac{w_1}{w_2}$ is rational

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 3.4.5. *Suppose that G_1 is a rational-weighted Hadamard diagonalizable graph. Denote by lcm the least common multiple of the denominators of its edge weights, and by gcd the greatest common divisor of all the new integer edge weights $lcm \cdot w(j,k)$. Then G_1 admits 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 $L(G_2) = \frac{lcm}{gcd} L(G_1)$ has PST at time $t_0 = \pi/2$ between the same pair of vertices (which can be checked through Theorem 3.4.2).*

Proof. The result follows directly from Remark 1.3.11. $\square$

Proposition 3.4.5 provides a way to extend Theorem 3.4.2 to a merge with rational weights. Assume that G_1 and G_2 are integer-weighted graphs. Assume that w_1 and w_2 are two nonzero real numbers such that $\frac{w_1}{w_2}$ is rational, say $\frac{w_1}{w_2} = \frac{p}{q}$ for two relatively prime numbers p and q. Then the PST property of $G_1 \; {}_{w_1}{\odot}_{w_2} \; G_2$ can be obtained from the PST property of the merge $G_1 \; {}_p{\odot}_q \; G_2$ of G_1 and G_2 with respect to integer weights p and q, as $L(G_1 \; {}_{w_1}{\odot}_{w_2} \; G_2) = \frac{w_2}{q} L(G_1 \; {}_p{\odot}_q \; G_2)$.

3.4.3 When $\frac{w_1}{w_2}$ is irrational

When $\frac{w_1}{w_2}$ is irrational, then the merge $G_1\ {}_{w_1}{\odot}_{w_2}\ G_2$ of two integer-weighted graphs G_1 and G_2 which have some PST properties as in Theorem 3.4.2, exhibits PGST. Before giving the theorem, we recall the following result about approximating an irrational real number with a sequence of rational numbers.

Theorem 3.4.6 ([81])**.** *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 p, q with $[p, q]$ in each of the three classes $[o, e]$, $[e, o]$, and $[o, o]$, such that the inequality $|w - p/q| < 1/q^2$ holds.*

Let G_1 and G_2 be regular graphs on n vertices. For the weighted graph $G_1\,{}_{w_1}{\odot}_{w_2}G_2$, we say that it has parameters $[w_1, w_2, d_2]$, where as in Theorem 3.4.2, d_2 denotes the degree of G_2. In particular, if w_1, w_2, and d_2 are all odd integers, then we say that the graph $G_1\,{}_{w_1}{\odot}_{w_2}G_2$ has type $[o, o, o]$. Similar notations apply for other possible parities of integers w_1, w_2 and d_2. We will denote the set of irrational numbers by $\mathbb{R}\backslash\mathbb{Q}$.

Theorem 3.4.7. *Assume that G_1 and G_2 are (labelled) integer-weighted graphs on n vertices, both of which are diagonalizable by the same normalized Hadamard matrix H. Let d_2 be the degree of G_2. Let $L(G_1)$ and $L(G_2)$ denote the Laplacian matrices of G_1 and G_2, respectively. Suppose that w_1 and w_2 are nonzero real numbers with $\frac{w_1}{w_2} \in \mathbb{R}\backslash\mathbb{Q}$. Let $j, k \in \{1, \ldots, n\}$.*

1. *Suppose that G_1 has PST from j to k at time $\pi/2$. Then $G_1\ {}_{w_1}{\odot}_{w_2}\ G_2$ has PGST*

from j to k and from $j+n$ to $k+n$.

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

3. *Suppose that the weighted graph with Laplacian $L(G_1)+L(G_2)$ has PST from j to k at time $\pi/2$. If d_2 is even, then $G_1\ {}_{w_1}\odot_{w_2} G_2$ has PGST from j to k and from $j+n$ to $k+n$. If d_2 is odd, then $G_1\ {}_{w_1}\odot_{w_2} G_2$ has PGST from j to $k+n$ and from k to $j+n$.*

Before proving this result, we note that it can alternatively be proved via Kronecker's theorem using the techniques from [7]. However, this would require proving that vertices j and k 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. By the scaling argument as in Remark 1.3.11, it can be assumed that $w_1 = 1$ and $w_2 \in \mathbb{R}\backslash\mathbb{Q}$, since for any non-zero real numbers w_1 and w_2, $L(G_1\ {}_{w_1}\odot_{w_2} G_2) = w_1 L(G_1\ {}_1\odot_{\frac{w_2}{w_1}} G_2)$.

We approximate w_2 with fractions p/q such that

$$|w_2 - p/q| < 1/q^2. \tag{3.6}$$

For each such pair of p, q, we denote the weighted graph $G_1\ {}_1\odot_{p/q} G_2$ as G_4, and the weighted graph $G_1\ {}_0\odot_{w_2-p/q} G_2$ as G_5. In particular, $L(G_1\ {}_1\odot_{w_2} G_2) = L(G_4)+L(G_5)$.

Now consider the integer-weighted graph $G_4' = G_1 \,{}_q\!\odot_p G_2$, then its Laplacian is $L(G_4') = qL(G_4)$ and has parameters $[q, p, d_2]$.

There are now a number of cases to consider. If $[p, q]$ is of type $[o, e]$ and d_2 is even, the graph G_4' is of type $[e, o, e]$. From Theorem 3.4.2 we know, if G_2 has PST from j to k at $\pi/2$, then G_4' has PST at $\pi/2$ from j to k and from $j+n$ to $k+n$ (Case 1(b), 2(b)). If $[p, q]$ is of type $[o, e]$ and d_2 is odd, then the graph G_4' is of type $[e, o, o]$. From Theorem 3.4.2 we know that if G_2 has PST at $\pi/2$ from j to k at $\pi/2$, then G_4' has PST at $\pi/2$ from j to $k+n$ and from k to $j+n$ (Case 3(a)).

If $[p, q]$ is of type $[e, o]$, then the weighted graph G_4' is of type $[o, e, f]$, where f denotes the parity of d_2. From Theorem 3.4.2 we know that if G_1 has PST from j to k at $\pi/2$, then G_4' has PST at $\pi/2$ from j to k and from $j+n$ to $k+n$ (Case 1(a), 2(a)).

If $[p, q]$ is of type $[o, o]$ and d_2 is even, then the graph G_4' is of type $[o, o, e]$. From Theorem 3.4.2 we know that if the graph with Laplacian $L(G_1) + L(G_2)$ has PST from j to k at $\pi/2$, then G_4' has PST from j to k and from $j+n$ to $k+n$ (Case 1(c), 2(c)). If $[p, q]$ is of type $[o, o]$ and d_2 is odd, then the graph G_4' is of type $[o, o, o]$. From Theorem 3.4.2 we know that if the integer weighted graph with Laplacian $L(G_1) + L(G_2)$ has PST from j to k at $\pi/2$, then G_4' has PST from j to $k+n$ and from k to $j+n$ (Case 3(b)).

For all the above cases, G_4 has PST at time $t_0 = q\pi/2$. Next, we make use of the following result from [52, Theorem 4] (Theorem 6.2.1 in Chapter 6) : Suppose PST occurs in the graph with Laplacian matrix L between vertices j and k at time $t = t_0$ and assume that $\hat{L} = L + L_0$ due to a small nonzero edge-weight perturbation L_0. Then

$$1 - |e_j^T e^{it_0 \hat{L}} e_k|^2 \leq 2|||t_0 L_0|||_2 + |||t_0 L_0|||_2^2 - |||t_0 L_0|||_2^3. \tag{3.7}$$

Note that the proof of the above theorem (Theorem 6.2.1) is independent of the results of Chapter 3. Now, G_4 is a graph with PST between vertices u and v at time $t_0 = \frac{q\pi}{2}$, and $L(G_1\ {}_1\!\odot_{w_2} G_2) = L(G_4) + L(G_5)$. Then the fidelity of state transfer between the vertices u and v in $G_1\ {}_1\!\odot_{w_2} G_2$ satisfies

$$\begin{aligned}
|e_u^T e^{it_0 L(G_1\ {}_1\odot_{w_2} G_2)} e_v|^2 &\geq 1 - 2|||t_0 L(G_5)|||_2 - |||t_0 L(G_5)|||_2^2 + |||t_0 L(G_5)|||_2^3 \\
&\geq 1 - 2q(\pi/2)|w_2 - p/q|cn - (2q(\pi/2)|w_2 - p/q|cn)^2 \\
&\quad + (2q(\pi/2)|w_2 - p/q|cn)^3 \\
&\geq 1 - 2cn\pi/(2q) - (cn\pi/(2q))^2 + (cn\pi/(2q))^3,
\end{aligned}$$

where $c = \max_{j,k} \left|(L(G_2))_{j,k}\right|$, and the last two inequalities come from Theorem 2.1.7 and (3.6), respectively. Since there are infinitely many integers q that satisfy (3.6), the expression on the right hand side in the above inequality can be made as close to 1 as possible by taking large enough q, and therefore $G_1\ {}_{w_1}\!\odot_{w_2} G_2$ admits PGST between vertices u and v. $\square$

3.4.4 An irrational-weighted graph exhibiting PGST from one vertex to three different vertices

It is known (Proposition 2.6.5) that if there is perfect state transfer from vertex j to vertex $k\,(\neq j)$ at time t_0, and perfect state transfer from vertex j to vertex $\ell\,(\neq j)$ at time t_1, then necessarily $k = \ell$. The following example, which is a straightforward consequence of Theorem 3.4.7, 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 3.4.8. Consider the graphs G_1, G_2 with the following Laplacian matrices (see Figure 3.3):

$$L(G_1) = \begin{bmatrix} 3 & -1 & -1 & 0 & -1 & 0 & 0 & 0 \\ -1 & 3 & 0 & -1 & 0 & -1 & 0 & 0 \\ -1 & 0 & 3 & -1 & 0 & 0 & -1 & 0 \\ 0 & -1 & -1 & 3 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 3 & -1 & -1 & 0 \\ 0 & -1 & 0 & 0 & -1 & 3 & 0 & -1 \\ 0 & 0 & -1 & 0 & -1 & 0 & 3 & -1 \\ 0 & 0 & 0 & -1 & 0 & -1 & -1 & 3 \end{bmatrix},$$

which has PST at time $\pi/2$ for the pairs $\{1, 8\}, \{2, 7\}, \{3, 6\}, \{4, 5\}$, and

$$L(G_2) = \begin{bmatrix} 3 & 0 & -1 & -1 & -1 & 0 & 0 & 0 \\ 0 & 3 & -1 & -1 & 0 & -1 & 0 & 0 \\ -1 & -1 & 3 & 0 & 0 & 0 & -1 & 0 \\ -1 & -1 & 0 & 3 & 0 & 0 & 0 & -1 \\ -1 & 0 & 0 & 0 & 3 & 0 & -1 & -1 \\ 0 & -1 & 0 & 0 & 0 & 3 & -1 & -1 \\ 0 & 0 & -1 & 0 & -1 & -1 & 3 & 0 \\ 0 & 0 & 0 & -1 & -1 & -1 & 0 & 3 \end{bmatrix}$$

which has PST at time $\pi/2$ for the pairs $\{1, 6\}, \{2, 5\}, \{3, 8\}, \{4, 7\}$.

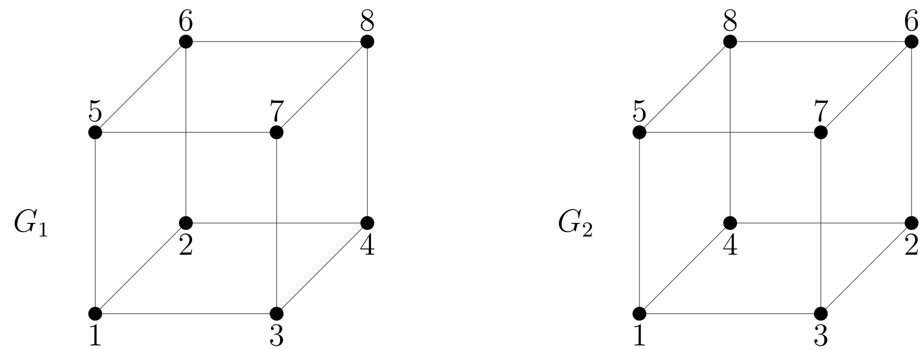


Figure 3.3: Graphs G_1 and G_2

It turns out that the weighted graph with Laplacian $L(G_1) + L(G_2)$ has PST at time $\pi/2$ between the pairs $\{1, 3\}, \{2, 4\}, \{5, 7\}, \{6, 8\}$. From the collection of cases in Theorem 3.4.7, we find that if $\frac{w_1}{w_2} \in \mathbb{R}\backslash\mathbb{Q}$, then $G_1 \ {}_{w_1}\!\odot_{w_2} G_2$ has the intriguing property that there is PGST between the pairs $\{1, 8\}, \{1, 11\}, \{1, 14\}$ (among others).

3.5 Optimality

3.5.1 Timing errors

In [52] (see Chapter 6), 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 are given in the most general setting where no information is known about the graph in question. Specifically, suppose that a graph G on n vertices admits Laplacian PST from vertex j to vertex k at time t_0. Suppose further that there is a small perturbation so that the readout time is instead $t_0 + h$, where $|h| < \frac{\pi}{\lambda_n}$ with λ_n being the largest eigenvalue of $L(G)$. Decompose the Laplacian matrix as $L(G) = Q\Lambda Q^T$, where $\Lambda = \operatorname{diag}(\lambda_1 = 0, \lambda_2, \ldots, \lambda_n)$, with $0 = \lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$, and Q is an orthogonal matrix of corresponding eigenvectors. If q_j and q_k are the j-th and k-th columns of Q^T, respectively, then for some $\theta \in \mathbb{R}$ we have $e^{i\theta} q_j = e^{it_0\Lambda} q_k$. Setting $B = \operatorname{diag}(e^{ih\lambda_1}, \ldots, e^{ih\lambda_n}) e^{i\theta}$, it follows that the fidelity at the perturbed time $t_0 + h$ is

$$\begin{aligned} p_{j,k}(t_0+h) &= |e_j^T e^{i(t_0+h)L(G)} e_k|^2 = |e_j^T Q e^{i(t_0+h)\Lambda} Q^T e_k|^2 \\ &= |q_j^T e^{i(t_0+h)\Lambda} q_k|^2 = |q_j^T e^{ih\Lambda} e^{it_0\Lambda} q_k|^2 \\ &= |q_j^T e^{ih\Lambda} e^{i\theta} q_j|^2 = |q_j^T B q_j|^2. \end{aligned}$$

In the special case that G is diagonalizable by a Hadamard matrix H, $Q = \frac{1}{\sqrt{n}} H$, and we can say more:

$$|q_j^T B q_j| = \frac{1}{n} \left| \sum_{\ell=1}^{n} e^{ih\lambda_\ell} \right|. \tag{3.8}$$

This suggests that, in order to maximize $|q_j^T B q_j|$, the goal should be to make the numbers $e^{ih\lambda_\ell}$ as closely-spaced on the complex unit circle as possible. This remark is not surprising but rather confirms the known rule [59] while at the same time providing a more accurate bound (in fact it is the fidelity) on timing errors for Hadamard diagonalizable graphs.

3.5.2 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 graphs with PST is the r-cube, which has 2^r vertices and degree r. We now show that if we restrict our attention to Hadamard diagonalizable unweighted graphs with PST, then for $r \leq 4$ the r-cube is indeed the sparsest connected graph with PST. After Theorem 3.6.2 we will see that if we restrict ourselves to graphs diagonalizable by the standard Hadamard matrix H_r, then the r-cube is indeed the sparsest such graph for any positive integer r.

Theorem 3.5.1. *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. The result follows by computing some quantities of the form $\mathrm{Tr}(L(G)^k)$ ($k \geq 0$ is an integer) in two different ways. First, let $\lambda_1 = 0, \ldots, \lambda_n$ denote the eigenvalues of $L(G)$, then $\mathrm{Tr}(L(G)^k) = \sum_{j=1}^{n} \lambda_j^k$. From $L(G) = rI - A(G)$, we know $\mathrm{Tr}(L(G)) = rn - \mathrm{Tr}(A(G))$ and $\mathrm{Tr}(L(G)^2) = r^2 n - 2r\mathrm{Tr}(A(G)) + \mathrm{Tr}(A(G)^2)$. Since G is a simple graph, we know that $\mathrm{Tr}(A(G)) = 0$ and it is straightforward to compute $\mathrm{Tr}(A(G)^2) = rn$. Thus we have the following system of equations:

$$\sum_{j=1}^{n} \lambda_j = \mathrm{Tr}(L(G)) = rn \quad \text{and} \quad \sum_{j=1}^{n} \lambda_j^2 = \mathrm{Tr}(L(G)^2) = rn(r+1).$$

Let c_λ denote the multiplicity of $\lambda \neq 0$ as an eigenvalue of $L(G)$ (with the convention that if λ is not an eigenvalue, then $c_\lambda = 0$). From Theorem 3.2.1 we know that all the λ_js are even integers, and we know by the Gershgorin circle theorem (Theorem 2.1.1) that $0 \leq \lambda_j \leq 2r$ for each j. Therefore the above equations tell us that

$$\sum_{j=0}^{r}(2j)c_{2j} = \sum_{j=1}^{r}(2j)c_{2j} = rn \quad \text{and} \quad \sum_{j=0}^{r}(2j)^2c_{2j}\sum_{j=1}^{r}(2j)^2c_{2j} = rn(r+1). \tag{3.9}$$

If we add in the equation $\sum_{j=1}^{r} c_{2j} = n-1$ (since 0 is a simple eigenvalue of the Laplacian of a connected graph), 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 by Theorem 3.2.2 and the fact that any two rows of a Hadamard matrix have half of the corresponding entries of the same sign, and half of the opposite sign, we know that half of $L(G)$'s eigenvalues must belong to each of the two even 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 equations (3.9) together with the equation $c_2 + c_6 = c_4 + c_8 + 1$ (again, because the even eigenvalues are split evenly between the two even 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 $\mathrm{Tr}(L(G)^3)$ in two different ways (similar to the way we did at the start of the proof): $\mathrm{Tr}(L(G)^3) = \sum_{j=1}^{n} \lambda_j^3 = r^3n - 3r^2\mathrm{Tr}(A(G)) + 3r\mathrm{Tr}(A(G)^2) - \mathrm{Tr}(A(G)^3) = r^3n + 3r^2n - \mathrm{Tr}(A(G)^3)$. Since $\mathrm{Tr}(A(G)^3) \geq 0$ we arrive at the inequality $\sum_{j=1}^{n} \lambda_j^3 \leq r^2n(r+3)$, which is equivalent to

$\sum_{j=1}^{r}(2j)^3c_{2j} \leq r^2n(r+3)$. Setting $r = 4$ 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 3.5.1 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 3.5.1 to the $r = 5$ case, we might try computing $\mathrm{Tr}(L(G)^4)$ in two different ways. However, we then end up with an equation involving both $-\mathrm{Tr}(A(G)^3)$ and $+\mathrm{Tr}(A(G)^4)$, and it is not clear how to bound such a quantity.

3.6 Cubelike graphs

3.6.1 Characterization of graphs diagonalizable by a standard Hadamard matrix

It is known that the adjacency matrix of any cubelike graph (and hence the Laplacian matrix, since cubelike graphs are regular) is diagonalizable by the standard Hadamard matrix [15]. The following result provides the converse; in the proof, the graph (possibly containing loops) with adjacency matrix A is denoted by $\Gamma(A)$ for convenience.

Lemma 3.6.1. *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: $\begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}$, $\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$, $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$. For these matrices, conclusions (1)–(3) follow readily.

Suppose that the result holds for some $k \in \mathbb{N}$ and that A is diagonalized by the standard Hadamard matrix $H_{k+1} = \begin{bmatrix} H_k & H_k \\ H_k & -H_k \end{bmatrix}$ of order 2^{k+1}. 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 $A_1 - A_2 = X - X^T = O$ by making use of the $(1,2)$ and $(2,1)$ blocks. Therefore $A_1 = A_2$, $X = X^T$, and the $(1,1)$ and $(2,2)$ blocks of the above equation imply that H_k diagonalizes both $2(A_1 + X)$ and $2(A_1 - X)$, and we conclude that H_k diagonalizes both A_1 and X. In particular, the induction hypothesis applies to A_1 and X. Thus A_1 has constant diagonal, and so does A (hence $\Gamma(A)$ is in fact $\Gamma(A_1) \odot \Gamma(X)$ if the diagonal of A_1 is 0).

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, either X has zero diagonal and so $\Gamma(X)$ 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 $C_2 = \tilde{C_2} \cup \{\mathbf{0}\}$ for the latter case.

We label the vertices of the graph $\Gamma(A)$ with vectors in $\mathbb{Z}_2^{k+1}$ in increasing lexicographic 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 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 $(k+1)$-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). $\square$

Note that the above proof shows that the merge of two n-cubelike graphs (both diagonalizable by H_n) is a cubelike graph.

Corollary 3.6.2. *Let G be an unweighted graph. Then $L(G)$ is diagonalized by a standard Hadamard matrix if and only if G is a cubelike graph.*

Proof. If $L(G)$ is diagonalizable by the standard Hadamard matrix, then in particular G is regular by Theorem 3.2.1. Hence the adjacency matrix of G is diagonalizable by the standard Hadamard matrix, so by Lemma 3.6.1, G is cubelike. Conversely, if G is cubelike, then it is regular and its adjacency matrix is diagonalizable by the standard Hadamard matrix [15]. Therefore $L(G)$ is diagonalizable by the standard Hadamard matrix. $\square$

The following result gives the PST property of the specially weighted n-cube at time $\pi/2$, generalizing the known fact that the unweighted hypercube graph has PST at time $\pi/2$.

Corollary 3.6.3. *Suppose that $w_1, w_2, \ldots, w_n$ are nonzero integers, exactly d of which are odd, and consider the weighted hypercube $\mathcal{C}_n := (w_1K_2)\square(w_2K_2)\square\cdots\square(w_nK_2)$. For each vertex u of $\mathcal{C}_n$, there is a vertex v at distance d from u such that there is perfect state transfer in $\mathcal{C}_n$ from u to v at time $t_0 = \pi/2$.*

It can be proved by induction and Theorem 2.2.5.

3.6.2 Uniform mixing on $(n+1)$-regular and $(n+2)$-regular connected cubelike graphs

The results in this section are independent from the paper [58], and are original to this thesis.

As mentioned previously, quantum information transfer properties of the n-cube $Q_n = K_2^{\square n}$ are straightforward to check by using the fact that $e^{itA(Q_n)} = (e^{itA(K_2)})^{\otimes n} = \begin{bmatrix} \cos(t) & i\sin(t) \\ i\sin(t) & \cos(t) \end{bmatrix}^{\otimes n}$ (by Theorem 2.2.6), where $B^{\otimes n}$ denotes the tensor product of B with itself for n times. Apart from PST, PGST, and FR, there is another interesting phenomenon in quantum information state transfer, called uniform mixing.

Definition 3.6.4. *Let G be a graph on n vertices with Hamiltonian $\mathcal{H}$. If there is a time t such that the fidelity $p_{j,k}(t)$ is the same for any $j, k \in \{1, 2, \ldots, n\}$, then we say that G admits* uniform mixing *at time t.*

From the fact that $U(t)$ is a unitary matrix, we know that if a graph G on n vertices admits uniform mixing at time t, then $p_{j,k}(t) = \frac{1}{n}$ for all $j, k \in \{1, \ldots, n\}$.

Since cubelike graphs are regular, such graphs admit adjacency uniform mixing if and only if they admit Laplacian uniform mixing (Proposition 1.3.10). We state our result in terms of the adjacency matrix without loss of generality. Since $e^{i\frac{\pi}{4}A(Q_n)} = (e^{i\frac{\pi}{4}A(K_2)})^{\otimes n} = \begin{bmatrix} \frac{1}{\sqrt{2}} & i\frac{1}{\sqrt{2}} \\ i\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix}^{\otimes n}$, we know that for any positive integer n, the n-cube admits uniform mixing at time $\frac{\pi}{4}$. Families of graphs with uniform mixing are known. Cubelike graphs with uniform mixing at time $\frac{\pi}{2^k}$ and cubelike graphs with PST at time $\frac{\pi}{2^k}$ are given in [25]. A complete characterization of all $2(d+2)$-regular Cayley graphs over $\mathbb{Z}_3^d$ that admit uniform mixing at time $\frac{2\pi}{9}$ is given [50]; also, for any $k \geq 3$, Cayley graphs over $\mathbb{Z}_q^d$ that admit uniform mixing at a faster time $\frac{2\pi}{q^k}$ with $q = 3, 4$ are constructed.

A connected n-regular cubelike graph G on 2^n vertices is isomorphic to the n-cube Q_n, through a bijection between the connection set of G and the connection set C_0 of Q_n — namely, the set of standard basis vectors of $\mathbb{Z}_2^n$. Without loss of generality, we consider the n-cubelike graphs obtained from the n-cube by adding some other elements to the connection set, and characterize when such $(n+1)$ or $(n+2)$-regular graphs admit uniform mixing at time $\frac{\pi}{4}$.

From [15, 29] we know that for any $u = u_1u_2\cdots u_n \in \mathbb{Z}_2^n$, the map $x \mapsto x+u$ is an automorphism of $\mathbb{Z}_2^n$, and it can be represented by a $2^n \times 2^n$ permutation matrix $P_u = \otimes_{j=1}^n R^{u_i}$, where $R = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. Note that each row and each column of P has exactly one 1. Now we index the rows and columns of P_u by the vectors in $\mathbb{Z}_2^n$, arranged in increasing lexicographic order. Assume that the j-th row/column has index x, and the k-th row/column has index $x+u$. Then for $e_j, e_k \in \mathbb{R}^{2^n}$, we have $P_ue_j = e_k$, Also, for any $u, v \in \mathbb{Z}_2^n$, $P_uP_v = P_{u+v} = P_vP_u$. Furthermore, if $C \subset \mathbb{Z}_2^n \setminus \{\mathbf{0}\}$ and G is a cubelike graph with connection set C, then $A(G) = \sum_{u\in C} P_u$, and $U_G(t) = e^{itA(G)} = e^{it\sum_{u\in C} P_u} = \prod_{u\in C} e^{itP_u} = \prod_{u\in C}(\cos(t)I + i\sin(t)P_u)$. For any $x \in \mathbb{Z}_2^n$, let $wt(x)$ denote the number of 1s in x.

Recall from Remark 2.5.1 that, if we order the vertices of Q_n according to the bipartition $V(Q_n) = V_1 \cup V_2$, then the adjacency matrix is of the form $A(Q_n) = \begin{bmatrix} 0 & B \\ B^T & 0 \end{bmatrix}$ for some $2^{n-1} \times 2^{n-1}$ matrix B, and the unitary matrix $U_{Q_n}(t) = e^{itA(Q_n)}$ can be written as $U_{Q_n}(t) = \begin{bmatrix} M_1(t) & iK(t) \\ iK^T(t) & M_2(t) \end{bmatrix}$ for some real matrices $M_1(t), M_2(t)$ and $K(t)$. Combined with the fact that Q_n admits uniform mixing at time $\frac{\pi}{4}$, we know that all the entries of $U_{Q_n}(\frac{\pi}{4})$ are either $\pm\frac{1}{2^{\frac{n}{2}}}$ or $\pm\frac{i}{2^{\frac{n}{2}}}$, i.e., $2^{\frac{n}{2}}M_1(\frac{\pi}{4}), 2^{\frac{n}{2}}M_2(\frac{\pi}{4})$ and $2^{\frac{n}{2}}K(\frac{\pi}{4})$ are all $(1,-1)$ matrices.

Now we consider adding one extra nonzero element $v \in \mathbb{Z}_2^n \setminus C_0$ to C_0, so we get a $(n+1)$-regular graph G_1. From the above analysis we know that at time $\frac{\pi}{4}$, the corresponding unitary matrix is $U_{G_1}(\frac{\pi}{4}) = e^{i\frac{\pi}{4}A(G_1)} = e^{i\frac{\pi}{4}\left(\sum_{u\in C_0} P_u + P_v\right)} = e^{i\frac{\pi}{4}\left(\sum_{u\in C_0} P_u\right)}e^{i\frac{\pi}{4}P_v} =$

$U_{Q_n}(\frac{\pi}{4})(\cos(\frac{\pi}{4})I + i\sin(\frac{\pi}{4})P_v) = \frac{\sqrt{2}}{2}U_{Q_n}(\frac{\pi}{4})(I + iP_v)$. Then G_1 admits uniform mixing at time $\frac{\pi}{4}$ if and only if all the entries of $2^{\frac{n}{2}}U_{Q_n}(\frac{\pi}{4})(I+iP_v)$ have modulus $\sqrt{2}$, which is true if and only if all the entries are in the set $\{1+i, 1-i, -1+i, -1-i\}$. Since $e_j^T 2^{\frac{n}{2}} U_{Q_n}(\frac{\pi}{4})(I+iP_v)e_k = 2^{\frac{n}{2}}\left(e_j^T U_{Q_n}(\frac{\pi}{4})e_k + ie_j^T U_{Q_n}(\frac{\pi}{4})P_v e_k\right) = 2^{\frac{n}{2}}\left(e_j^T U_{Q_n}(\frac{\pi}{4})e_k + ie_j^T U_{Q_n}(\frac{\pi}{4})e_\ell\right)$, where if the k-th row/column of P_v has index x then the ℓ-th row/column of P_v has index $x+v$, therefore all the entries of $2^{\frac{n}{2}}U_{Q_n}(\frac{\pi}{4})(I+iP_v)$ are in the set $\{1+i, 1-i, -1+i, -1-i\}$ if and only if the map $x \mapsto x+v$ is a bijection of V_1 to itself (and a bijection of V_2 to itself) (where $V_1 = \{x \in \mathbb{Z}_2^n \mid wt(x) \equiv 0 \pmod 2\}$ and $V_2 = \{x \in \mathbb{Z}_2^n \mid wt(x) \equiv 1 \pmod 2\}$ are the two sets of the bipartition of $V(Q_n)$), which means that G_1 is not bipartite. From the construction of V_1 and V_2, we know G_1 is not bipartite if and only if $wt(v) \equiv 0 \pmod 2$. We summarize these observations in the following result.

Proposition 3.6.5. *Suppose that we add an extra nonzero element $v \in \mathbb{Z}_2^n \setminus C_0$ to the connection set $C_0 = \{e_1, \dots, e_n\}$ of Q_n to get a new cubelike graph G_1. Then the following are equivalent:*

- *G_1 admits uniform mixing at time $\frac{\pi}{4}$,*
- *G_1 is not bipartite,*
- *$wt(v) \equiv 0 \pmod 2$.*

Hence if we add one extra element v to the connection set of a connected n-regular n-cubelike graph (isomorphic to Q_n, but the connection set might not be C_0), then the new graph admits uniform mixing at time $\frac{\pi}{4}$ if and only if the resulting graph is not bipartite.

Example 3.6.6. Adding $v = 0101$ to the connection set $C_0 = \{e_1, e_2, e_3, e_4\}$ of the 4-cube, gives a non-bipartite 4-cubelike graph that admits uniform mixing at time $\frac{\pi}{4}$, since $wt(v) \equiv 0 \pmod 2$. Adding $u = 1101$ to the connection set $C_0 = \{e_1, e_2, e_3, e_4\}$ of the 4-cube, gives a bipartite 4-cubelike graph that does not admit uniform mixing at time $\frac{\pi}{4}$, since $wt(u) \equiv 1 \pmod 2$.

Making use of the fact that cubelike graphs are diagonalizable by the standard Hadamard matrix, we can get the spectral decomposition of a cubelike graph, and with the method shown in Remark 2.1.3, we can get a closed form formula for e^{itA}, where A is the adjacency matrix of a cubelike graph. This can be used to confirm the above results obtained from Proposition 3.6.5.

Now we consider adding two extra nonzero elements to the connection set C_0 of Q_n. Again we order the vertices of Q_n in the increasing lexicographic order of the binary numbers in $\mathbb{Z}_2^n$. Denote the matrix $\begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}$ by F, then $U_{Q_n}(\frac{\pi}{4}) = \frac{1}{2^{\frac{n}{2}}}(F^{\otimes n})$, where $F^{\otimes n}$ denotes the tensor product of F with itself for n times.

Now for $u, v \in \mathbb{Z}_2^n$, we give a formula for the (u, v)-entry of $2^{\frac{n}{2}} U_{Q_n}(\frac{\pi}{4})$, and for the (u, v)-entry of the permutation matrix P_w for $w \in \mathbb{Z}_2^n$. In the following, the sum $u_j + v_j$ is performed in $\mathbb{Z}_2$, and the sum $u + v$ is performed in $\mathbb{Z}_2^n$. For an integer p, let $[p]_2$ denote the remainder when p is divided by 2.

Proposition 3.6.7. *Let n be a positive integer. For $u, v, w \in \mathbb{Z}_2^n$, we have $2^{\frac{n}{2}}(U_{Q_n}(\frac{\pi}{4}))_{u,v} = i^{wt(u+v)}$, and $(P_w)_{u,v} = 1$ if and only if $u + v = w$.*

Proof. When $n = 1$, for $u, v \in \mathbb{Z}_2$, the (u, v) entry of $F = \begin{bmatrix} 1 & i \\ i & 1 \end{bmatrix}$ is $i(-i)^{[u+v+1]_2}$, which satisfies the above formula. For $n \geq 1$, assume $u = u_1 u_2 \cdots u_n$, $v = v_1 v_2 \cdots v_n$, and let $S_0 = \{j = 1, \ldots, n | u_j = v_j = 0\}$, $S_1 = \{j = 1, \ldots, n | u_j = v_j = 1\}$. Then

$$\begin{aligned}
\left(2^{\frac{n}{2}}\left(U_{Q_n}\left(\frac{\pi}{4}\right)\right)\right)_{u,v} &= (F^{\otimes n})_{u,v} \\
&= (i(-i)^{[u_1+v_1+1]_2})(i(-i)^{[u_2+v_2+1]_2}) \cdots (i(-i)^{[u_n+v_n+1]_2}) \\
&= i^n(-i)^{|S_0|+|S_1|} \\
&= i^n(-i)^{n-wt(u+v)} \qquad \text{(as } wt(u+v) = n - |S_0| - |S_1|) \\
&= (i(-i))^n(-i)^{-wt(u+v)} \\
&= i^{wt(u+v)}.
\end{aligned}$$

Similarly for $P_w = R^{w_1} \otimes R^{w_2} \otimes \cdots \otimes R^{w_n}$, we have $(P_w)_{u,v} = ([u_1+v_1+w_1+1]_2)([u_2+v_2+w_2+1]_2) \cdots ([u_n+v_n+w_n+1]_2)$, which equal to 1 if and only if $[u_j+v_j+w_j]_2 = [0]_2$ for all $j = 1, \ldots, n$, i.e., $u+v = w$. Therefore for the permutation matrix P_w, and $u \in \mathbb{Z}_2^n$, the only nonzero entry in the u-th row of P_w is the $(u, u+w)$-entry. $\square$

Now consider adding two nonzero elements $u, v \in \mathbb{Z}_2^n \setminus C_0$ to the connection set C_0 of the n-cube. For two elements $u, v \in \mathbb{Z}_2^n$, we say the pair (u, v) is of type (a, b, c) for $a, b, c \in \{0, 1\}$, if $wt(u) \equiv a \pmod 2, wt(v) \equiv b \pmod 2, [u \cap v] \equiv c \pmod 2$, where $[u \cap v]$ denotes $|\{j = 1, \ldots, n | u_j = v_j = 1\}|$.

Theorem 3.6.8. *Assume we get an $(n+2)$-regular n-cubelike graph G_2 by adding two nonzero elements $u, v \in \mathbb{Z}_2^n \setminus C_0$ to the connection set C_0 of the n-cube. Then G_2 admits* *uniform mixing at time $\frac{\pi}{4}$ if and only if (u,v) is of one of the following four types:* $(0,0,0)$*,* $(0,1,1)$*,* $(1,0,1)$*, and* $(1,1,1)$*.*

Proof. We find $U_{G_2}(\frac{\pi}{4}) = e^{i\frac{\pi}{4}\left((\sum_{x\in C_0} P_x)+P_u+P_v\right)} = e^{i\frac{\pi}{4}\left(\sum_{x\in C_0} P_x\right)} e^{i\frac{\pi}{4}P_u} e^{i\frac{\pi}{4}P_v} = U_{Q_n}(\frac{\pi}{4})(\cos(\frac{\pi}{4})I + i\sin(\frac{\pi}{4})P_u)(\cos(\frac{\pi}{4})I + i\sin(\frac{\pi}{4})P_v) = \frac{1}{2}U_{Q_n}(\frac{\pi}{4})(I+iP_u)(I+iP_v) = \frac{1}{2}U_{Q_n}(\frac{\pi}{4})(I - P_{u+v} + i(P_u+P_v))$. G_2 admits uniform mixing at time $\frac{\pi}{4}$ if and only if all the entries of $U_{G_2}(\frac{\pi}{4})$ have modulus $\frac{1}{2^{\frac{n}{2}}}$, i.e., all the entries of $\tilde{U} = 2^{\frac{n}{2}}U_{Q_n}(\frac{\pi}{4})(I - P_{u+v} + i(P_u+P_v))$ have modulus 2, which happens exactly when the entries of $\tilde{U}$ are of the form ± 2 or $\pm 2i$, since all the entries of $2^{\frac{n}{2}}U_{Q_n}(\frac{\pi}{4})$ are ± 1 or $\pm i$.

Denote the matrix $2^{\frac{n}{2}}U_{Q_n}(\frac{\pi}{4})$ by $\hat{U}$. For $x,y\in\mathbb{Z}_2^n$, $\tilde{U}_{x,y} = \hat{U}_{x,y} - (\hat{U}P_{u+v})_{x,y} + i(\hat{U}P_u)_{x,y} + i(\hat{U}P_v)_{x,y} = i^{wt(x+y)} - \hat{U}_{x,y+u+v} + i\hat{U}_{x,y+u} + i\hat{U}_{x,y+v} = i^{wt(x+y)} - i^{wt(x+y+u+v)} + i\cdot i^{wt(x+y+u)} + i\cdot i^{wt(x+y+v)} = i^{wt(w)} - i^{wt(w+u+v)} + i\cdot i^{wt(w+u)} + i\cdot i^{wt(w+v)}$, where $w = x+y$. Using the fact that for any $x,y\in\mathbb{Z}_2^n$, $wt(x+y) = wt(x)+wt(y)-2[x\cap y]$, the above equation can be rewritten as

$$\begin{aligned}
\tilde{U}_{x,y} &= i^{wt(w)} - i^{wt(w)+wt(u+v)-2[w\cap(u+v)]} + i^{wt(w)+wt(u)-2[w\cap u]+1} + i^{wt(w)+wt(v)-2[w\cap v]+1} \\
&= i^{wt(w)}(1 - i^{wt(u)+wt(v)-2[u\cap v]-2([w\cap u]+[w\cap v]-2[w\cap u\cap v])} + i^{wt(u)-2[w\cap u]+1} + i^{wt(v)-2[w\cap v]+1}) \\
&= i^{wt(w)}(1 - i^{wt(u)+wt(v)-2[u\cap v]-2[w\cap u]-2[w\cap v]} + i^{wt(u)-2[w\cap u]+1} + i^{wt(v)-2[w\cap v]+1}) \\
&= i^{wt(w)}(1 - i^{wt(u)+wt(v)}(-1)^{[u\cap v]+[w\cap u]+[w\cap v]} + i^{wt(u)+1}(-1)^{[w\cap u]} + i^{wt(v)+1}(-1)^{[w\cap v]}).
\end{aligned}$$

Hence G_2 admits uniform mixing at time $\frac{\pi}{4}$ if and only if $a = 1 + i^{wt(u)+1}(-1)^{[w\cap u]} + i^{wt(v)+1}(-1)^{[w\cap v]} - i^{wt(u)+wt(v)}(-1)^{[u\cap v]+[w\cap u]+[w\cap v]}$ has modulus 2 for all $w\in\mathbb{Z}_2^n$.

- If $[u\cap v]\equiv 0 \pmod 2$, then $a = 1 - i^{wt(u)+wt(v)}(-1)^{[w\cap u]+[w\cap v]} + i^{wt(u)+1}(-1)^{[w\cap u]} + i^{wt(v)+1}(-1)^{[w\cap v]} = \left(1 + i^{wt(u)+1}(-1)^{[w\cap u]}\right)\left(1 + i^{wt(v)+1}(-1)^{[w\cap v]}\right)$, and $|a| = 2$ if and only if each of the two factors has modulus $\sqrt{2}$, which is true if and only if $wt(u) \equiv 0 \pmod{2}$ and $wt(v) \equiv 0 \pmod{2}$. This gives us the type $(0, 0, 0)$.

- If $[u \cap v] \equiv 1 \pmod{2}$, then $a = 1 + i^{wt(u)+wt(v)}(-1)^{[w\cap u]+[w\cap v]} + i^{wt(u)+1}(-1)^{[w\cap u]} + i^{wt(v)+1}(-1)^{[w\cap v]} = 2 - \left(1 - i^{wt(u)+1}(-1)^{[w\cap u]}\right)\left(1 - i^{wt(v)+1}(-1)^{[w\cap v]}\right)$, and $|a| = 2$ if and only if one of the two factors has modulus 0 or 2, which is true if and only if $wt(u) \equiv 1 \pmod{2}$ or $wt(v) \equiv 1 \pmod{2}$. This gives us the three types $(0, 1, 1)$, $(1, 0, 1)$ and $(1, 1, 1)$.

$\square$

Example 3.6.9. Adding elements $u = 01110$ and $v = 10010$ to the connection set $C_0 = \{e_1, \ldots, e_5\}$ of the 5-cube produces a 5-cubelike graph that admits uniform mixing at time $\frac{\pi}{4}$, as $[u \cap v] \equiv 1 \pmod{2}$, $wt(u) \equiv 1 \pmod{2}$, $wt(v) \equiv 0 \pmod{2}$, and therefore (u, v) is of type $(1, 0, 1)$. Similarly, adding elements $u = 00110$ and $v = 10110$ to the connection set $C_0 = \{e_1, \ldots, e_5\}$ of the 5-cube produces a 5-cubelike graph that does not admit uniform mixing at time $\frac{\pi}{4}$, as $[u \cap v] \equiv 0 \pmod{2}$, $wt(u) \equiv 0 \pmod{2}$, $wt(v) \equiv 1 \pmod{2}$, and therefore (u, v) is of type $(0, 1, 0)$.

Chapter 4

Perfect quantum state transfer in weighted paths with loops using orthogonal polynomials

Among connected graphs on n vertices, the path is one of the graphs that has a simple structure, and it realizes the largest possible diameter. As mentioned in Chapter 1, the unweighted path on n vertices only exhibits adjacency PST for $n \leq 3$, and only exhibits Laplacian PST for $n \leq 2$. A natural generalization is to consider weighted paths. Christandl, Datta, Dorlas, Ekert, Kay and Landahl [30] showed that adjacency PST can be achieved over arbitrarily long distances by using a specific set of edge weights; the edge weights they used to achieve adjacency PST from vertex 1 to vertex n were $w_{j,j+1} = \sqrt{j(n-j)}$ for each $j \in \{1, \ldots, n-1\}$. Another generalization is to add weighted loops on the vertices of an unweighted path. It is true that if there are two non-adjacent vertices u and v in a graph G such that u and v share the same neighbours, then adding properly weighted loops on the vertices of G will help achieve PST between u and v [63]. However, there is no such set of weighted loops to add on the vertices of an unweighted path on $n \geq 4$ vertices to achieve adjacency PST between the end vertices.

A further generalization is to consider weighted paths with weighted loops. Kay [61] found a necessary and sufficient condition on the eigenvalues for a weighted mirror-symmetric path with loops to exhibit PST between its end vertices at a given time t_0. Given a set of n distinct real numbers (a real-weighted path has only simple and real eigenvalues) satisfying certain conditions (for example, to ensure PST for a weighted path), several algorithms exist [37] [43, Chapter 4] [86] for constructing a tridiagonal matrix (corresponding to a weighted path with or without loops) that has those numbers as eigenvalues (and therefore exhibits PST).

In this chapter, we consider weighted paths on n vertices, with vertex set $\{1, 2, \cdots, n\}$, from a matrix analysis point of view: weighted paths with loops (potentials) amount to tridiagonal matrices (a matrix $A = [a_{j,k}]$ is called tridiagonal if $a_{j,k} = 0$ whenever $|j-k| > 1$) with certain restrictions (e.g. the diagonal entries of the adjacency matrix of a weighted path (without loops) are necessarily zero). Any symmetric tridiagonal matrix gives way to a three-term recurrence relation, and a finite sequence of polynomials defined by a three-term recurrence relation is a sequence of orthogonal polynomials, so our approach is to work with the orthogonal polynomials (see Section 4.1.1 for more details) that arise by considering the tridiagonal matrix as an operator on the polynomial space.

In Section 4.1, we review some basic results about orthogonal polynomials, three-term recurrences, and a necessary and sufficient condition on the eigenvalues of a weighted path with or without loops to exhibit PST between the end vertices at a given time t_0. Based on this, we give some observations to simplify the analysis in the following sections. In Section 4.2, using an approach similar to that found in [41], we obtain formulas, in terms of eigenvalues, for the weight of the edge between vertices $\left\lfloor \frac{n}{2} \right\rfloor$ and $\left\lfloor \frac{n}{2}+1 \right\rfloor$ and of the loop at vertex $\left\lceil \frac{n}{2} \right\rceil$. This allows one to determine the "middle" weights of the weighted path with loops with a given spectrum without the need to calculate all the orthogonal polynomials or the weights of the inner product. In Section 4.3, we give the main result: any weighted path on $n \geq 3$ vertices does not admit Laplacian PST between the two end vertices, nor do certain mirror symmetric trees between their symmetric vertex pairs. In Section 4.4, we propose the following conjecture: weighted paths on at least four vertices with or without loops must have at least one irrational weight in order to have adjacency PST between the end vertices at the fixed readout time π; we confirm this conjecture for $n = 4$ as well as for $n \equiv 3 \pmod 8$ and for $n \equiv 5 \pmod 8$.

Throughout this chapter, in the setting of adjacency matrices, we consider paths with or without loops; in the Laplacian matrix setting, we only consider paths without loops. This chapter is based on work with Kirkland, McLaren, Pereira and Plosker [67]. The work began when Pereira visited the University of Manitoba in June 2017 for a one-week period. McLaren was Plosker's undergraduate student research assistant in Summer 2017.

4.1 Preliminaries

4.1.1 Orthogonal polynomials and three-term recurrence

In this section, we review some basics about orthogonal polynomials; for more details, see [44, Chapter 8].

The set of all real polynomials in one real variable forms a vector space $\mathcal{P}$. If μ is a measure on $\mathbb{R}$ such that $\int x^{2n} d\mu < \infty$ for all non-negative integers n, then we can define an inner product on this vector space by $(p, q) := \int p(x)q(x)d\mu$. Given this inner product we can find an orthogonal basis $(p_j)_{j\geq 0}$ for $\mathcal{P}$ such that p_j is a polynomial of degree j. We say that $(p_j)_{j\geq 0}$ is a sequence of *orthogonal polynomials*.

The factors and zeros of each polynomial in a sequence of orthogonal polynomial have some nice properties.

Theorem 4.1.1 ([44], Lemma 8.1.1)**.** *Let $(p_j)_{j\geq 0}$ be a sequence of orthogonal polynomials. Suppose that for some $n \geq 0$, a polynomial f is a proper factor of p_n. If f is nonnegative, then it must be constant.*

Therefore we have the following.

Corollary 4.1.2 ([44], Section 8.1)**.** *Let $(p_j)_{j\geq 0}$ be a sequence of orthogonal polynomials. Then for any $n \geq 0$, all the roots of $p_n(x)$ are real, and they are all simple roots.*

Orthogonal polynomials are closely related to three-term recurrence relations.

Theorem 4.1.3 ([44], Theorem 8.2.1)**.** *Let* $(p_j)_{j\geq 0}$ *be a sequence of monic orthogonal polynomials and set*

$$a_j = \frac{(xp_j, p_j)}{(p_j, p_j)}, \quad b_j = \frac{(p_j, p_j)}{(p_{j-1}, p_{j-1})}.$$

Then for all positive integers j*,*

$$p_{j+1}(x) = (x - a_j)p_j(x) - b_j p_{j-1}(x). \tag{4.1}$$

A recurrence of the form

$$xp_j(x) = B_j p_{j+1}(x) + A_j p_j(x) + C_j p_{j-1}(x)$$

with the product $B_j C_j$ being a positive real number for all j, is known as a *three-term recurrence*. If we extend our sequence of orthogonal polynomials by defining p_{-1} to be the zero polynomial, then the three-term recurrence in the above theorem holds for all nonnegative integers j.

On the other hand, three-term recurrence relations also give rise to orthogonal polynomials.

Theorem 4.1.4 ([44], Corollary 8.4.3)**.** *A finite sequence of polynomials defined by a three-term recurrence is a sequence of orthogonal polynomials.*

One consequence of Theorem 4.1.3 is the following.

Corollary 4.1.5 ([44], Section 8.2)**.** *Let* $(p_j)_{j\geq 0}$ *be a sequence of orthogonal polynomials. Then the polynomials* $p_{n+1}(x)$ *and* $p_n(x)$ *have no non-trivial common factor, whenever* $n \geq 0$.

The following result connects the adjacency matrix or Laplacian matrix of a weighted or unweighted path with or without loops to the theory of orthogonal polynomials.

Proposition 4.1.6 ([44], Corollary 8.2.2)**.** *The orthogonal polynomial $p_{n+1}(x)$ satisfying equation (4.1) with $p_{-1} = 0$, and $p_0 = 1$ (and $j = n$) is the characteristic polynomial of the symmetric matrix*

$$B_{n+1} = \begin{bmatrix} a_0 & \sqrt{b_1} & & & \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & & \ddots & & \\ & & \sqrt{b_{n-1}} & a_{n-1} & \sqrt{b_n} \\ & & & \sqrt{b_n} & a_n \end{bmatrix}.$$

Proof. We proceed by induction on n. If $n \leq 1$, the result is immediate. If $n \geq 1$, then we expand $\det(xI_{n+1} - B_{n+1})$ along the last row to obtain

$$\begin{aligned} \det(xI_{n+1} - B_{n+1}) &= (x - a_n)\det(xI_n - B_n) - b_n \det(xI_{n-1} - B_{n-1}) \\ &= (x - a_n)p_n(x) - b_n p_{n-1}(x). \end{aligned}$$

This yields the desired result. □

Corollary 4.1.7 ([44], Section 8.2)**.** *Let $(p_j)_{j\geq 0}$ be a sequence of orthogonal polynomials. The the zeros of p_{n+1} interlace the zeros of p_n for any $n > 0$.*

Proof. From Proposition 4.1.6, we know that the zeros of any orthogonal polynomial are the eigenvalues of the adjacency matrix of a weighted path with loops. Combining this fact with Theorem 2.1.15, we obtain the desired result. □

Now given the adjacency matrix or Laplacian matrix of a weighted path, we find the associated finite sequence of orthogonal polynomials, the associated sequence of monic orthogonal polynomials, as well as a tridiagonal matrix associated to this finite monic orthogonal polynomial sequence, then we use them to find the eigenvectors associated to the two matrices, which will be used to study the quantum state transfer property of paths.

4.1.2 Paths and orthogonal polynomials

Here we focus on two settings: weighted paths governed by Laplacian dynamics, and weighted paths, that may or may not have loops, governed by adjacency dynamics. In both settings, the vertices of the path are labelled so that vertex j is adjacent to vertex $j+1, j = 1, \ldots, n-1$. As a result, the Hamiltonian will always be a tridiagonal matrix of one of the following two forms depending on the dynamics.

$$A = \begin{bmatrix} q_1 & r_1 & & & & \\ r_1 & q_2 & r_2 & & & \\ & r_2 & q_3 & r_3 & & \\ & & & \ddots & & \\ & & & & & r_{n-1} \\ & & & & r_{n-1} & q_n \end{bmatrix}, L = \begin{bmatrix} q_1 & -r_1 & & & & \\ -r_1 & q_2 & -r_2 & & & \\ & -r_2 & q_3 & -r_3 & & \\ & & & \ddots & & \\ & & & & & -r_{n-1} \\ & & & & -r_{n-1} & q_n \end{bmatrix} \tag{4.2}$$

where $r_j > 0$ denotes the weight of the edge between vertex j and $j+1$. For the adjacency matrix case, all $q_j = 0$ for (unweighted or weighted) paths without loops. The weight of the loop at vertex j corresponds a nonzero entry q_j. For the Laplacian matrix case, as we are only considering weighted or unweighted paths (without loops), it follows that $q_1 = r_1$, $q_j = r_{j-1} + r_j$ for $j = 2, 3, \ldots, n-1$, and $q_n = r_{n-1}$.

Expanding $\det(xI_n - A)$ (or $\det(xI_n - L)$) along the last row and making use of Theorem 4.1.4, we note that both of the two symmetric tridiagonal $n \times n$ matrices in (4.2) are connected to a set of n orthogonal polynomials via the three-term recurrence given by

$$p_k(x) = (x - q_k)p_{k-1}(x) - r_{k-1}^2 p_{k-2}(x) \quad \text{for all } k \in \{1, \ldots, n\}, \tag{4.3}$$

where $p_k(x)$ denotes the characteristic polynomial of the leading principal submatrix of A or L of size k (note that we have the same recurrence relation for the sequence of orthogonal polynomials associated to A or L). Further we define $p_{-1}(x) = 0$ and $p_0(x) = 1$, and denote the eigenvalues of A or L (that is, the roots of $p_n(x)$) by α_r, $r = 1, \ldots, n$.

Rearranging equation (4.3), we find that $xp_{k-1}(x) = p_k(x)+q_k p_{k-1}(x)+r_{k-1}^2 p_{k-2}(x)$. Combined with the fact that $p_{-1}(x) = 0$ and $p_0(x) = 1$, it follows that $(p_j(x))_{j=0,1,\ldots,n}$ is a sequence of monic orthogonal polynomials and satisfy

$$xp_{k-1}(x) = p_k(x) + q_k p_{k-1}(x) + r_{k-1}^2 p_{k-2}(x) \text{ for } k = 0, 1, \ldots, n. \tag{4.4}$$

Consider the matrix

$$X = \begin{bmatrix} q_1 & 1 & & & & \\ r_1^2 & q_2 & 1 & & & \\ & r_2^2 & q_3 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & r_{n-2}^2 & q_{n-1} & 1 \\ & & & & r_{n-1}^2 & q_n \end{bmatrix}. \tag{4.5}$$

Equation (4.4) implies that the matrix X represents multiplication by $x \pmod{p_n(x)}$ in the basis $\mathcal{B} = \{p_0(x), \ldots, p_{n-1}(x)\}$:

$$X \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} \equiv x \begin{bmatrix} p_0(x) \\ p_1(x) \\ \vdots \\ p_{n-1}(x) \end{bmatrix} \pmod{p_n(x)}. \tag{4.6}$$

We note that A is similar to X via $QX = AQ$ where $Q = \operatorname{diag}(d_1, \ldots, d_n)$ and

$$d_j = \begin{cases} \dfrac{1}{\prod_{\ell=1}^{j-1} r_\ell} & \text{if } j \neq 1, \\ 1 & \text{if } j = 1. \end{cases} \tag{4.7}$$

The matrix L is also similar to X via $TX = LT$ where $T = \mathrm{diag}\,(d_1, \ldots, d_n)$ and

$$d_j = \begin{cases} \dfrac{(-1)^{j-1}}{\prod_{\ell=1}^{j-1} r_\ell} & \text{if } j \neq 1, \\ 1 & \text{if } j = 1. \end{cases} \tag{4.8}$$

Let M denote the matrix A or L in equation (4.2). From the discussions at the beginning of this section and Corollary 4.1.2, we know that the eigenvalues of M are real and distinct, since $r_j > 0$ for all $j = 1, \ldots, n-1$. We then use this distinctness to order the eigenvalues as follows:

$$\alpha_1 < \alpha_2 < \cdots < \alpha_n. \tag{4.9}$$

Since X is similar to M, we know that $\alpha_1, \ldots, \alpha_n$ are all the eigenvalues of X. Note that an eigenvector of X associated to the eigenvalue α_j is

$$w_j = [p_0(\alpha_j),\ p_1(\alpha_j),\ \cdots,\ p_{n-1}(\alpha_j)]^T.$$

This can be verified by computing Xw_j, and then using the recurrence relation (4.4) evaluated at α_j to simplify each term (keep in mind $p_n(\alpha_j) = 0$ for $j = 1, \ldots, n$), or we can use equation (4.6) directly.

Now, let us consider the set of polynomials $S = \{\tilde{p}_0(x), \ldots, \tilde{p}_{n-1}(x)\}$ with $\tilde{p}_k(x) = d_{k+1}p_k(x)$, where the d_ks are given by equation (4.7) if we are taking $M = A$ and the d_ks are given by equation (4.8) if we are taking $M = L$. As with the set $\mathcal{B}$, the set S is also a basis of the vector space of all polynomials of degree less than n. In the basis S, the matrix that represents multiplication by the $x \pmod{p_n(x)}$ is exactly M:

$$M \begin{bmatrix} \tilde{p}_0(x) \\ \tilde{p}_1(x) \\ \vdots \\ \tilde{p}_{n-1}(x) \end{bmatrix} \equiv x \begin{bmatrix} \tilde{p}_0(x) \\ \tilde{p}_1(x) \\ \vdots \\ \tilde{p}_{n-1}(x) \end{bmatrix} \quad (\text{mod } p_n(x)).$$

Let $v_j = [\tilde{p}_0(\alpha_j), \tilde{p}_1(\alpha_j), \ldots, \tilde{p}_{n-1}(\alpha_j)]^T$. Then v_j is an eigenvector of M associated to the eigenvalue α_j, since from $M = \tilde{Q}X\tilde{Q}^{-1}$ and $Xw_j = \alpha_j w_j$, we know that an eigenvector v_j for M corresponding to the eigenvalue α_j is $v_j = \tilde{Q}w_j = [d_1 p_0(\alpha_j), \cdots, d_n p_{n-1}(\alpha_j)]^T$, with $\tilde{Q} = Q$ if $M = A$, and $\tilde{Q} = T$ if $M = L$. Therefore the two vectors v_r and v_s are orthogonal to each other for any $r \neq s$ (eigenvectors of a real symmetric matrix associated to distinct eigenvectors are orthogonal to each other).

Normalizing these vectors, assume the normalization factors are $\sqrt{\kappa_j}$ (in fact, $\kappa_j = \frac{1}{v_j^T v_j}$), $j = 1, \ldots, n$, respectively, then the matrix $V = [\sqrt{\kappa_1} v_1, \sqrt{\kappa_2} v_2, \ldots, \sqrt{\kappa_n} v_n]$ is an orthogonal matrix, and it diagonalizes the Hamiltonian $\mathcal{H} = M$ to the diagonal matrix $\Lambda = \operatorname{diag}(\alpha_1, \ldots, \alpha_n)$, i.e., $V^T M V = \Lambda$.

4.1.3 Characterization of the eigenvalues of a weighted path with or without loops that exhibits PST at time π

Let V and Λ be the two matrices as in the previous section. Recall that V is real orthogonal and Λ is diagonal such that $V^T M V = \Lambda$. Denote the ℓ-th row of V by r_ℓ, $\ell = 1, \ldots, n$. Proposition 2.6.2 tells us that there is PST between vertex j and k at time $t = t_0$ if and only if $r_j e^{it_0\Lambda} = e^{i\phi} r_k$ for some phase factor ϕ. If $p_{j-1}(\alpha_r) \neq 0$ for $r = 1, \ldots, n$, then the vector equality can be rewritten as

$$\frac{\tilde{p}_{k-1}(\alpha_r)}{\tilde{p}_{j-1}(\alpha_r)} = e^{-i\phi} e^{it_0\alpha_r} \tag{4.10}$$

for $r = 1, 2, \ldots, n$. Since the polynomials $\tilde{p}_\ell(x)$ are real, it follows that $\tilde{p}_{k-1}(\alpha_r)/\tilde{p}_{j-1}(\alpha_r) = \pm 1$. In particular, if we consider the case of PST between the end vertices of the corresponding weighted path, i.e., $j = 1$ and $k = n$, then, combining the fact that $\tilde{p}_{j-1}(x) = \tilde{p}_0(x) = p_0(x) = 1$ for all x with the interlacing property of zeros of $p_n(x)$ and $p_{n-1}(x)$ from Corollary 4.1.7, it can be shown [86] that

$$\tilde{p}_{n-1}(\alpha_r) = (-1)^{n+r}. \tag{4.11}$$

Therefore $e^{-i\phi} e^{it_0\alpha_r} = (-1)^{n+r}$. Looking at two neighbouring eigenvalues α_r and α_{r-1}, we can see that $e^{it_0(\alpha_r - \alpha_{r-1})} = -1$ and therefore $\alpha_r - \alpha_{r-1} = (2m_r + 1)\pi/t_0$ for some nonnegative integer m_r [61]. Now we scale the Hamiltonian (A or L depending on the dynamics) by a factor t_0/π so that the PST time is π, and we therefore look at a simpler expression

$$\alpha_r - \alpha_{r-1} = 2m_r + 1. \tag{4.12}$$

By Lemma 2.6.3, for a system with symmetric tridiagonal Hamiltonian $\mathcal{H} = M$, if PST occurs between the end vertices, then M is persymmetric (symmetric about the anti-diagonal; persymmetric matrices are also called mirror symmetric or Hankel symmetric in the literature). Combining these results together, we obtain the following result.

Corollary 4.1.8. *A weighted path (with loops) with eigenvalues $\alpha_1, \ldots, \alpha_n$ admits PST between its end vertices at time π if and only if the Hamiltonian $\mathcal{H} = M$ is persymmetric and the eigenvalues $\alpha_1, \ldots, \alpha_n$ satisfy equation (4.12).*

In the case of a weighted path having no loops, the associated graph is then bipartite, and therefore the eigenvalues of the adjacency matrix (A with $q_1 = \cdots = q_n = 0$) are symmetric about zero (Theorem 3.14 [9]). In this case, we give the eigenvalues another set of labels as follows

$$-\beta_{\frac{n}{2}} < \cdots < -\beta_2 < -\beta_1 < 0 < \beta_1 < \beta_2 < \cdots < \beta_{\frac{n}{2}}, \text{ for } n \text{ even}$$
$$-\beta_{\frac{n-1}{2}} < \cdots < -\beta_2 < -\beta_1 < \beta_0 = 0 < \beta_1 < \beta_2 < \cdots < \beta_{\frac{n-1}{2}}, \text{ for } n \text{ odd} \qquad (4.13)$$

(we use zero as the index of the zero eigenvalue in the case that n is odd; zero does not appear as an eigenvalue in the case when n is even). From now on, when we mention the eigenvalues as α_r, we mean the ones ordered as in (4.9), and when we mention eigenvalues β_r we mean the ones as in (4.13). If n is even then (4.12) and (4.13) yield the fact that $\beta_1 - (-\beta_1) = 2\beta_1 = (2m_1 + 1)$, and therefore $\beta_1 = (2m_1 + 1)/2$. Using this, we find

$$\begin{aligned} \beta_2 - \beta_1 &= (2m_2 + 1) \\ \Rightarrow \beta_2 &= (2m_2 + 1) + \frac{(2m_1 + 1)}{2} \\ &= \frac{(4m_2 + 2m_1 + 3)}{2}. \end{aligned}$$

Following this, we see that if n is even, all β_r will be odd multiples of $1/2$. In fact, one can easily show by continuing the analysis of $\beta_r - \beta_{r-1}$, that β_rs alternate between $1 \pmod 4$

times $1/2$ and $3 \pmod 4$ times $1/2$ (these give us alternating $\pm i$ when considering $e^{i\pi\beta_r}$ in the matrix exponential $e^{i\pi M}$). A similar analysis shows that if n is odd, then β_rs are integers, alternating between even and odd (these give us alternating ± 1 when considering $e^{i\pi\beta_r}$), with $\beta_0 = 0$. We summarize this in the following remark:

Remark 4.1.9. A weighted mirror-symmetric path without loops exhibits adjacency PST between its end vertices at time π if and only if its eigenvalues β_r adhere to the following pattern: for n even, β_rs alternate between $(1 \bmod 4) \times 1/2$ and $(3 \bmod 4) \times 1/2$, while for n odd, β_rs alternate between even and odd integers.

For the adjacency matrix of a weighted path with loops, we can shift all the eigenvalues (by adding a multiple of the identity matrix) such that the smallest eigenvalue is an integer; equation (4.12) then tells us that the eigenvalues α_js must alternate between even and odd. This new weighted path with loops will exhibit PST between its end vertices if and only if the original one does, by Proposition 1.3.9. Therefore the eigenvalues can then be assumed to be integers with alternating parity without loss of generality. For a weighted path without loops, its Laplacian matrix L is positive semi-definite with smallest eigenvalue 0 (of multiplicity 1, since the graph is connected). Using this together with equation (4.12), we know that the integer sequence of ordered eigenvalues α_r begins with 0 (even number) and then alternates odd, even, odd, ... for all the remaining eigenvalues. We summarize this in the following remark:

Remark 4.1.10. A weighted mirror-symmetric path with loops (with adjacency matrix A) exhibits adjacency PST between its end vertices at time π if and only if for some scalar matrix aI, the shifted adjacency matrix $A + aI$ has its eigenvalues α_r alternating between odd and even integers (with the odd-indexed eigenvalues being odd integers, and the even-indexed eigenvalues being even integers). A weighted mirror-symmetric path with no loops exhibits Laplacian PST between its end vertices at time π, if and only if the Hamiltonian $\mathcal{H} = L$ has its eigenvalues α_r alternate between even and odd integers (starting with the smallest eigenvalue: zero).

Note that for a weighted path with or without loops that admits PST between its end vertices (not necessarily at time π), we can always scale the Hamiltonian so that PST occurs at time π, and use Remark 4.1.9 and Remark 4.1.10 to obtain a pattern for the eigenvalues of the scaled system, which provides a pattern for the eigenvalues of the original system.

Now we check the relation of occurrence of PST between internal vertices and between the two end vertices on a weighted path.

Proposition 4.1.11. *For a weighted path with or without loops on n vertices, PST between vertices 1 and n implies PST between vertices j and $n+1-j$, for each $j = 2, \ldots, n-1$. If for some j with $2 \leq j \leq n-1$, a weighted mirror-symmetric path on n vertices admits PST between vertices j and $n+1-j$, and if in addition none of the eigenvectors of the Hamiltonian $\mathcal{H} = M$ has a zero entry in the j–th position (i.e., for the orthogonal polynomial sequence $(p_\ell(x))_{\ell=0,1,\ldots,n}$ associated to the tridiagonal matrix M, for each eigenvalue α_r of $p_n(x)$, $p_{j-1}(\alpha_r) \neq 0$), then the converse holds.*

Proof. We have shown in Section 4.1.2 that an eigenvector v_r of M associated to the eigenvalue α_r is

$$\begin{aligned} v_r &= Qw_r \quad (\text{or } v_r = Tw_r \text{ if } M = L) \\ &= \begin{bmatrix} d_1 p_0(\alpha_r) \\ \vdots \\ d_n p_{n-1}(\alpha_r) \end{bmatrix} = \begin{bmatrix} \tilde{p}_0(\alpha_r) \\ \vdots \\ \tilde{p}_{n-1}(\alpha_r) \end{bmatrix}. \end{aligned} \tag{4.14}$$

Now, if we assume that there is PST between the end vertices, then M is persymmetric (Lemma 2.6.3), that is, $RMR = M$ (or $RM = MR$), where R denotes the reversal matrix, which has 1s on the anti-diagonal and 0s elsewhere. Now $Mv_r = \alpha_r v_r$ implies that $M(Rv_r) = R(Mv_r) = R(\alpha_r v_r) = \alpha_r(Rv_r)$. Since $Rv_r \neq 0$, this means that Rv_r is an eigenvector of M associated to the eigenvalue α_r. The facts that α_r is a simple eigenvalue and that $\|Rv_r\|_2 = \|v_r\|_2$ imply that $Rv_r = \pm v_r$. Hence the eigenvectors v_r of M are either symmetric or antisymmetric, i.e $(v_r)_j = \pm(v_r)_{n-j+1}$, $j = 1, 2, \ldots, n$, therefore either $\tilde{p}_{j-1}(\alpha_r)$ and $\tilde{p}_{n-j}(\alpha_r)$ are both zero, or neither of them is zero and for some phase factor $\hat{\phi}$, as shown in equation (4.10) they satisfy

$$\frac{\tilde{p}_{j-1}(\alpha_r)}{\tilde{p}_{n-j}(\alpha_r)} = \frac{\tilde{p}_0(\alpha_r)}{\tilde{p}_{n-1}(\alpha_r)} = e^{i(\pi\alpha_r - \hat{\phi})} = \pm 1. \tag{4.15}$$

The above is valid for all α_r and j such that $\tilde{p}_{n-j}(\alpha_r) \neq 0$, and the quotients share the same alternating pattern between 1 and -1 determined by PST between the end vertices; hence there is perfect state transfer between the vertices j and $n+1-j$ (as $r_j e^{it_0 M} = e^{i\hat{\phi}} r_{n+1-j}$ in this case).

The steps above are all reversible under certain conditions: if there is PST between a pair of inner vertices j and $n+1-j$ for some $2 \leq j \leq n-1$, and if $p_{j-1}(\alpha_r) \neq 0$ for all $r = 1, \ldots, n$ (and therefore $p_{n-j}(\alpha_r) \neq 0$ as well), then equation (4.15) is true for all α_r

and the given j, and therefore there is PST between the two end vertices. $\square$

Referring to the proof of Proposition 4.1.11, we observe in passing that if $p_{j-1}(\alpha_r) = p_{n-j}(\alpha_r) = 0$ for some r, then it does not provide the $e^{i(\pi\alpha_r - \hat{\phi})} = \pm 1$ constraints on the eigenvalues needed for PST between end vertices.

The following three sections contain the main results of [67].

4.2 Expressing the weight of the middle edge and of the middle loop of a weighted persymmetric tridiagonal matrix in terms of its eigenvalues

Given a set of n eigenvalues (with restrictions given from equation (4.12)), we would like to reconstruct the adjacency matrix of a weighted mirror-symmetric path with or without loops, that is guaranteed to have PST between vertices 1 and n. That is, by choosing values for $\alpha_1, \ldots, \alpha_n$ satisfying Equation (4.12) (these will correspond to the eigenvalues of the matrix), one can reverse-engineer weighted paths, with or without loops, having PST. We go through the low-dimensional cases in detail in this section and the next section.

First we state a technical result that is especially helpful in analyzing the eigenvalues of persymmetric matrices.

Lemma 4.2.1. [22, Lemma 3] *Let R be the* reversal matrix*: the anti-diagonal matrix with all ones along the antidiagonal.*

1. *If n is even, then the persymmetric matrix* $B = \begin{bmatrix} E & RCR \\ C & RER \end{bmatrix}$ *and the block diagonal matrix* $\begin{bmatrix} E-RC & 0 \\ 0 & E+RC \end{bmatrix}$ *are orthogonally similar, where E and C are any* $\frac{n}{2} \times \frac{n}{2}$ *matrices, and R is also* $\frac{n}{2} \times \frac{n}{2}$.

2. *If n is odd, then the persymmetric matrix* $B = \begin{bmatrix} E & x & RCR \\ x^T & q & x^T R \\ C & Rx & RER \end{bmatrix}$ *and the block diagonal matrix* $\begin{bmatrix} E-RC & 0 & 0 \\ 0 & q & \sqrt{2}x^T \\ 0 & \sqrt{2}x & E+RC \end{bmatrix}$ *are orthogonally similar, where E and C are any* $\frac{n-1}{2} \times \frac{n-1}{2}$ *matrices, R is also* $\frac{n-1}{2} \times \frac{n-1}{2}$, $q \in \mathbb{R}$, *and* $x \in \mathbb{R}^{\frac{n-1}{2}}$.

Applying Lemma 4.2.1 to the adjacency matrix of a mirror symmetric weighted path with or without loops, we can express the weight of the middle edge (and the weight of the loop on the middle vertex) in terms of the eigenvalues. Let $S_1 = \sum_{r=1}^{n}(-1)^{r+n}\alpha_r$ and $S_2 = \sum_{r=1}^{n}(-1)^{r+n}\alpha_r^2$.

Proposition 4.2.2. *Let A be the adjacency matrix of a weighted mirror-symmetric path with or without loops on n vertices, whose edge weights are as in (4.2). If n is even, then* $r_{\frac{n}{2}} = \dfrac{S_1}{2}$ *and* $q_{\frac{n}{2}} = \dfrac{S_2}{2S_1}$. *If n is odd, then* $r_{\frac{n-1}{2}} = \dfrac{\sqrt{S_2 - S_1^2}}{2}$ *and* $q_{\frac{n+1}{2}} = S_1$.

Proof. Suppose n is even. The adjacency matrix

$$A = \begin{bmatrix} q_1 & r_1 & & & & & & & & \\ r_1 & q_2 & r_2 & & & & & & & \\ & r_2 & q_3 & r_3 & & & & & & \\ & & & \ddots & & & & & & \\ & & & r_{\frac{n}{2}-1} & q_{\frac{n}{2}} & r_{\frac{n}{2}} & & & & \\ & & & & r_{\frac{n}{2}} & q_{\frac{n}{2}} & r_{\frac{n}{2}-1} & & & \\ & & & & & & \ddots & & & \\ & & & & & & & r_2 & q_2 & r_1 \\ & & & & & & & & r_1 & q_1 \end{bmatrix} \tag{4.16}$$

can be seen as a block matrix $A = \begin{bmatrix} E & RCR \\ C & RER \end{bmatrix}$ with $E = \begin{bmatrix} q_1 & r_1 & & \\ r_1 & q_2 & r_2 & \\ & & \ddots & \\ & & r_{\frac{n}{2}-1} & q_{\frac{n}{2}} \end{bmatrix}$ and $C = \begin{bmatrix} 0 & 0 & \cdots & 0 & r_{\frac{n}{2}} \\ 0 & 0 & \cdots & 0 & 0 \\ & & \ddots & & \\ 0 & & \cdots & 0 & 0 \end{bmatrix}$. By Lemma 4.2.1, A is orthogonally similar to the block diagonal matrix with diagonal blocks

$$B_1 = \begin{bmatrix} q_1 & r_1 & & & \\ r_1 & q_2 & r_2 & & \\ & r_2 & q_3 & r_3 & \\ & & & \ddots & \\ & & & r_{\frac{n}{2}-1} & (q_{\frac{n}{2}} - r_{\frac{n}{2}}) \end{bmatrix} \text{ and } B_2 = \begin{bmatrix} q_1 & r_1 & & & \\ r_1 & q_2 & r_2 & & \\ & r_2 & q_3 & r_3 & \\ & & & \ddots & \\ & & & r_{\frac{n}{2}-1} & (q_{\frac{n}{2}} + r_{\frac{n}{2}}) \end{bmatrix}.$$

Note that $B_2 = B_1 + 2r_{\frac{n}{2}} e_{\frac{n}{2}} e_{\frac{n}{2}}^T$. It is a well-known fact that if one perturbs a Hermitian matrix by a rank-one symmetric matrix, then the original matrix and the perturbed matrix will have interlacing eigenvalues (Theorem 2.1.11). Since $r_{\frac{n}{2}}$ is positive, it follows that B_1 has eigenvalues $\alpha_1, \alpha_3, \ldots, \alpha_{n-1}$ and B_2 has eigenvalues $\alpha_2, \alpha_4, \ldots, \alpha_n$, where $\alpha_1 < \alpha_2 < \ldots < \alpha_n$ are all the eigenvalues of A.

From the fact that the trace of a matrix is the sum of its eigenvalues, we find $2r_{\frac{n}{2}} = \mathrm{Tr}(B_2) - \mathrm{Tr}(B_1) = S_1$ and therefore $r_{\frac{n}{2}} = \dfrac{S_1}{2}$. Now, from the fact that the trace of the square of a matrix is the sum of the squares of the eigenvalues of the original matrix, we find that $(q_{\frac{n}{2}} + r_{\frac{n}{2}})^2 - (q_{\frac{n}{2}} - r_{\frac{n}{2}})^2 = \mathrm{Tr}(B_2^2) - \mathrm{Tr}(B_1^2) = S_2$, which simplifies to $4q_{\frac{n}{2}}r_{\frac{n}{2}} = S_2$. Therefore, $q_{\frac{n}{2}} = \frac{S_2}{2S_1}$.

Suppose n is odd. The adjacency matrix

$$A = \begin{bmatrix} q_1 & r_1 & & & & & & & & & \\ r_1 & q_2 & r_2 & & & & & & & & \\ & r_2 & q_3 & r_3 & & & & & & & \\ & & & \ddots & & & & & & & \\ & & & r_{\frac{n-1}{2}-1} & q_{\frac{n-1}{2}} & r_{\frac{n-1}{2}} & & & & & \\ & & & & r_{\frac{n-1}{2}} & q_{\frac{n+1}{2}} & r_{\frac{n-1}{2}} & & & & \\ & & & & & r_{\frac{n-1}{2}} & q_{\frac{n-1}{2}} & r_{\frac{n-1}{2}-1} & & & \\ & & & & & & & \ddots & & & \\ & & & & & & & & r_2 & q_2 & r_1 \\ & & & & & & & & & r_1 & q_1 \end{bmatrix} \quad (4.17)$$

is orthogonally similar to a block diagonal matrix with diagonal blocks

$$B_1 = \begin{bmatrix} q_1 & r_1 & & & \\ r_1 & q_2 & r_2 & & \\ & r_2 & q_3 & r_3 & \\ & & & \ddots & \\ & & & r_{\frac{n-1}{2}-1} & q_{\frac{n-1}{2}} \end{bmatrix} \text{ and } B_2 = \begin{bmatrix} q_{\frac{n+1}{2}} & 0 & \cdots & \sqrt{2}r_{\frac{n-1}{2}} \\ 0 & & & \\ \vdots & & B_1 & \\ \sqrt{2}r_{\frac{n-1}{2}} & & & \end{bmatrix}.$$

(Here, C is a zero matrix.) From Cauchy's interlacing theorem for a bordered Hermitian matrix (Theorem 2.1.15), we know the eigenvalues of B_1 are $\alpha_2, \alpha_4, \ldots, \alpha_{n-1}$, and the eigenvalues of B_2 are $\alpha_1, \alpha_3, \ldots, \alpha_n$. A trace argument similar to the even case yields $q_{\frac{n+1}{2}} = \mathrm{Tr}(B_2) - \mathrm{Tr}(B_1) = S_1$ and $q_{\frac{n+1}{2}}^2 + 4r_{\frac{n-1}{2}}^2 = \mathrm{Tr}(B_2^2) - \mathrm{Tr}(B_1^2) = S_2$. Therefore

$r_{\frac{n-1}{2}} = \frac{\sqrt{S_2 - S_1^2}}{2}$. □

Remark 4.2.3. For the Laplacian L of a weighted mirror-symmetric path (without loops) on n vertices, we have a similar result : if n is even, then $r_{\frac{n}{2}} = \dfrac{S_1}{2}$ and $q_{\frac{n}{2}} = \dfrac{S_2}{2S_1}$; if n is odd, then $r_{\frac{n-1}{2}} = \dfrac{\sqrt{S_2 - S_1^2}}{2}$ and $q_{\frac{n+1}{2}} = S_1$. Furthermore, for the even case, from $q_{\frac{n}{2}} = r_{\frac{n}{2}-1} + r_{\frac{n}{2}}$, we obtain $r_{\frac{n}{2}-1} = \frac{S_2 - S_1^2}{2S_1}$. For the odd case, from $q_{\frac{n+1}{2}} = 2r_{\frac{n-1}{2}}$, it follows that $S_2 = 2S_1^2$.

Example 4.2.4. Using Proposition 4.2.2, we will check what edge weight sets allow a weighted path on 2 or 3 vertices to admit PST between the end vertices.

For $n = 2$, Proposition 4.2.2 yields a weighted path with loops having $r_1 = \dfrac{\alpha_2 - \alpha_1}{2}$ and $q_1 = \dfrac{\alpha_2 + \alpha_1}{2}$. If we consider a weighted path with no loops (and so α_1, α_2 are simply $-\beta_1$, β_1 as in (4.13)), the Hamiltonian A reduces to $\begin{bmatrix} 0 & \beta_1 \\ \beta_1 & 0 \end{bmatrix}$. If $2\beta_1 = 2\ell + 1$ for some nonnegative integer ℓ, then Remark 4.1.9 implies that A admits PST between the two end vertices at time π, and therefore the unweighted path on two vertices, whose adjacency matrix is $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, admits PST from vertex 1 to vertex 2 at time $\beta_1 \pi = \frac{2\ell+1}{2}\pi$ by Remark 1.3.11, which is consistent with literature [45] (the unweighted path P_2 admits adjacency PST at time $t_0 = \frac{\pi}{2}$, and therefore also at $t = (2\ell + 1)t_0$ for any non-negative integer ℓ). Similarly, for the Laplacian case, since $\alpha_1 = 0$, the Hamiltonian L reduces to $\frac{1}{2}\begin{bmatrix} \alpha_2 & -\alpha_2 \\ -\alpha_2 & \alpha_2 \end{bmatrix}$. Again by Remark 4.1.9, if $\alpha_2 = 2\ell + 1$ for some nonnegative integer ℓ, then L admits PST at time π, and the unweighted path on 2 vertices admits Laplacian PST at time $\frac{2\ell+1}{2}\pi$.

For $n = 3$, Proposition 4.2.2 implies that a weighted path with loops, whose eigenvalues are α_1, α_2 and α_3, has weights $r_1 = \dfrac{\sqrt{-2\alpha_2^2 + 2\alpha_1\alpha_2 - 2\alpha_1\alpha_3 + 2\alpha_2\alpha_3}}{2}$ and $q_2 = \alpha_1 - \alpha_2 + \alpha_3$. Furthermore, since B_1 is simply the 1×1 matrix $[q_1]$, we can find q_1 via $q_1 = \mathrm{Tr}(B_1) = \alpha_2$.

Under adjacency dynamics, the Hamiltonian $\mathcal{H} = M$ is

$$A = \begin{bmatrix} \alpha_2 & \frac{\sqrt{-2\alpha_2^2+2\alpha_1\alpha_2-2\alpha_1\alpha_3+2\alpha_2\alpha_3}}{2} & 0 \\ \frac{\sqrt{-2\alpha_2^2+2\alpha_1\alpha_2-2\alpha_1\alpha_3+2\alpha_2\alpha_3}}{2} & \alpha_1 - \alpha_2 + \alpha_3 & \frac{\sqrt{-2\alpha_2^2+2\alpha_1\alpha_2-2\alpha_1\alpha_3+2\alpha_2\alpha_3}}{2} \\ 0 & \frac{\sqrt{-2\alpha_2^2+2\alpha_1\alpha_2-2\alpha_1\alpha_3+2\alpha_2\alpha_3}}{2} & \alpha_2 \end{bmatrix} \tag{4.18}$$

If we consider a weighted path with no loops (and so α_1, α_2, α_3 are simply $-\beta_1$, 0, β_1), the adjacency matrix reduces to

$$A = \begin{bmatrix} 0 & \frac{\beta_1}{\sqrt{2}} & 0 \\ \frac{\beta_1}{\sqrt{2}} & 0 & \frac{\beta_1}{\sqrt{2}} \\ 0 & \frac{\beta_1}{\sqrt{2}} & 0 \end{bmatrix}. \tag{4.19}$$

Again by Remark 4.1.9, if β_1 is an odd integer, say $\beta_1 = 2\ell + 1$ for some nonnegative integer ℓ, then A admits PST between vertices 1 and 3 at time π. Therefore Remark 1.3.11 implies that the unweighted path on 3 vertices admits adjacency PST at time $\frac{2\ell+1}{\sqrt{2}}\pi$, which is consistent with literature [45] (the unweighted path P_3 admits adjacency PST at time $t_0 = \frac{\pi}{\sqrt{2}}$). Similarly for the Laplacian dynamics, from Remark 4.2.3 and the fact that $\alpha_1 = 0$, we know the Laplacian reduces to

$$L = \begin{bmatrix} \alpha_2 & -\frac{\sqrt{-2\alpha_2^2+2\alpha_2\alpha_3}}{2} & 0 \\ -\frac{\sqrt{-2\alpha_2^2+2\alpha_2\alpha_3}}{2} & \alpha_3 - \alpha_2 & -\frac{\sqrt{-2\alpha_2^2+2\alpha_2\alpha_3}}{2} \\ 0 & -\frac{\sqrt{-2\alpha_2^2+2\alpha_2\alpha_3}}{2} & \alpha_2 \end{bmatrix}.$$

Since there are no loops on the weighted path, we have $\alpha_2 = \frac{\sqrt{-2\alpha_2^2+2\alpha_2\alpha_3}}{2}$ and $\alpha_3 - \alpha_2 = \sqrt{-2\alpha_2^2 + 2\alpha_2\alpha_3}$. Solving the two equations together, we obtain $\alpha_3 = 3\alpha_2$. By

Remark 4.1.9 (if a weighted path admits Laplacian PST at time π, then its eigenvalues alternate between even and odd integers), we know that a weighted path (without loops) on three vertices does not admit Laplacian PST.

4.3 PST between the end vertices of a weighted path fails for the Laplacian dynamics

The previous example shows that there are no weighted paths on 3 vertices that admit Laplacian PST between the end vertices. In fact, we have a more general result.

4.3.1 There is no Laplacian PST between the two end vertices of a weighted path on $n \geq 3$ vertices

As discussed in Remark 4.1.10, if there is Laplacian PST at time π between the end vertices of a weighted path (without loops), then the eigenvalues of the Laplacian are integers and alternate between even and odd (starting at zero).

Theorem 4.3.1. *No weighted (or unweighted) path on $n \geq 3$ vertices admits Laplacian PST between its end vertices.*

Proof. Assume a weighted path admits Laplacian PST between its end vertices; by a suitable scaling of the Laplacian we can assume that PST occurs at time π. Therefore the eigenvalues $\alpha_1 = 0 < \alpha_2 < \ldots < \alpha_n$ of the Laplacian are all integers and alternate between even and odd as mentioned in Remark 4.1.10. We begin with the case when n is even. The persymmetric Laplacian is of the form

$$L = \begin{bmatrix} r_1 & -r_1 & & & & & & & & \\ -r_1 & r_1+r_2 & -r_2 & & & & & & & \\ & -r_2 & r_2+r_3 & -r_3 & & & & & & \\ & & & \ddots & & & & & & \\ & & & -r_{\frac{n}{2}-1} & r_{\frac{n}{2}-1}+r_{\frac{n}{2}} & -r_{\frac{n}{2}} & & & & \\ & & & & -r_{\frac{n}{2}} & r_{\frac{n}{2}-1}+r_{\frac{n}{2}} & -r_{\frac{n}{2}-1} & & & \\ & & & & & & \ddots & & & \\ & & & & & & & -r_2 & r_1+r_2 & -r_1 \\ & & & & & & & & -r_1 & r_1 \end{bmatrix} \tag{4.20}$$

with E and C written according to Lemma 4.2.1. Then L is orthogonally similar to $\begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}$, where $B_1 = E - RC = \begin{bmatrix} r_1 & -r_1 & & & \\ -r_1 & r_1{+}_2 & -r_2 & & \\ & -r_2 & r_2+r_3 & -r_3 & \\ & & & \ddots & \\ & & & -r_{\frac{n}{2}-1} & (r_{\frac{n}{2}-1}+2r_{\frac{n}{2}}) \end{bmatrix}$, and $B_2 = E{+}RC = \begin{bmatrix} r_1 & -r_1 & & & \\ -r_1 & r_1{+}_2 & -r_2 & & \\ & -r_2 & r_2+r_3 & -r_3 & \\ & & & \ddots & \\ & & & -r_{\frac{n}{2}-1} & r_{\frac{n}{2}-1} \end{bmatrix}$. Note that the eigenvalues of B_1 are $\alpha_2, \cdots, \alpha_n$, and the eigenvalues of B_2 are $\alpha_1, \cdots, \alpha_{n-1}$.

Note that in this setting B_2 is the Laplacian matrix for the weighted path G on $\frac{n}{2}$ vertices with edge weights $r_j, j = 1, \ldots, \frac{n}{2} - 1$. Theorem 2.1.17 (part 2) tells us that all the principal minors of B_2 of size $\frac{n}{2} - 1$ are equal, and they are equal to the product $r_1 r_2 \cdots r_{\frac{n}{2}-1}$ of all the weights of the weighted path G, as G has only one spanning tree — itself. Recall that the eigenvalues of the Laplacian matrix B_2 are $\alpha_1 = 0, \alpha_3, \ldots, \alpha_{n-1}$;

part 1 of Theorem 2.1.17 implies that

$$\frac{n}{2}r_1 r_2 \cdots r_{\frac{n}{2}-1} = \alpha_3\alpha_5\cdots\alpha_{n-1}. \tag{4.21}$$

Now, we compute the determinant of B_1. Observe that B_1 can be written as $B_2 + 2r_{\frac{n}{2}}e_{\frac{n}{2}}e_{\frac{n}{2}}^T$, where as observed above, B_2 is the Laplacian matrix for a weighted path on $\frac{n}{2}$ vertices. Expanding the determinant along the last row (or column), we deduce that $\det B_1 = \det B_2 + 2r_{\frac{n}{2}}c$, where c is the leading principal minor of B_2 of order $\frac{n}{2} - 1$. Evidently $\det B_2 = 0$ (as it is the Laplacian matrix of a weighted path), and in the previous paragraph we have found that $c = r_1 r_2 \ldots r_{\frac{n}{2}-1}$; hence $\det B_1 = 2r_1 r_2 \cdots r_{\frac{n}{2}}$. Recall the eigenvalues of B_1 are $\alpha_2, \alpha_4, \ldots, \alpha_n$. The fact the product of all the eigenvalues of a matrix equals the determinant of the matrix implies that

$$2r_1 r_2 \cdots r_{\frac{n}{2}} = \alpha_2\alpha_4\cdots\alpha_n. \tag{4.22}$$

Combining equations (4.21) and (4.22), we find that

$$2r_{\frac{n}{2}} = \frac{\frac{n}{2}\alpha_2\alpha_4\cdots\alpha_n}{\alpha_3\alpha_5\cdots\alpha_{n-1}}. \tag{4.23}$$

Now, $2r_{\frac{n}{2}} = S_1 \in \mathbb{Z}$ by Proposition 4.2.2 and the fact that all α_js are integers. The numerator of the right hand side of equation (4.23) is $\frac{n}{2}$ times all the odd eigenvalues while the denominator is the product of all the even eigenvalues. Thus we obtain a factor of $2^{\frac{n}{2}-1}$ in the denominator, from which it follows that $2^{\frac{n}{2}-1}$ divides $\frac{n}{2}$, which is a contradiction provided $\frac{n}{2} \geq 3$, i.e. provided $n \geq 6$.

If $n = 4$, we have more information about $2r_2 = S_1 = \alpha_4 - \alpha_3 + \alpha_2 - \alpha_1$ — it is an even integer, as $\alpha_1 = 0$ and α_3 are even integers, and α_2, α_4 are odd integers. Then

(4.23), which simplifies to $2r_2 = \frac{2\alpha_2\alpha_4}{\alpha_3}$ in this case, implies that 4 divides 2, which is a contradiction. This completes the case of even n.

We now assume n is odd. The Hamiltonian is

$$L = \begin{bmatrix} r_1 & -r_1 & & & & & & & \\ -r_1 & r_1+r_2 & -r_2 & & & & & & \\ & & \ddots & & & & & & \\ & & -r_{\frac{n-1}{2}-1} & r_{\frac{n-1}{2}-1}+r_{\frac{n-1}{2}} & -r_{\frac{n-1}{2}} & & & & \\ & & & -r_{\frac{n-1}{2}} & 2r_{\frac{n-1}{2}} & -r_{\frac{n-1}{2}} & & & \\ & & & & -r_{\frac{n-1}{2}} & r_{\frac{n-1}{2}-1}+r_{\frac{n-1}{2}} & -r_{\frac{n-1}{2}-1} & & \\ & & & & & \ddots & & & \\ & & & & & -r_2 & r_1+r_2 & -r_1 \\ & & & & & & -r_1 & r_1 \end{bmatrix}, \tag{4.24}$$

and again we take E and $C = 0_{\frac{n}{2},\frac{n}{2}}$ as in Lemma 4.2.1. Then L is orthogonally similar to $\begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}$, where $B_1 = \begin{bmatrix} r_1 & -r_1 & & & \\ -r_1 & r_1+r_2 & -r_2 & & \\ & -r_2 & r_2+r_3 & -r_3 & \\ & & & \ddots & \\ & & & -r_{\frac{n-1}{2}-1} & (r_{\frac{n-1}{2}-1}+r_{\frac{n-1}{2}}) \end{bmatrix}$, and

$$B_2 = \begin{bmatrix} 2r_{\frac{n-1}{2}} & 0 & \cdots & \sqrt{2}r_{\frac{n-1}{2}} \\ 0 & & & \\ \vdots & & B_1 & \\ \sqrt{2}r_{\frac{n-1}{2}} & & & \end{bmatrix}.$$

The eigenvalues of B_1 and B_2 interlace, with $\sigma(B_1) = \{\alpha_2, \alpha_4, \ldots, \alpha_{n-1}\}$ and $\sigma(B_2) = \{\alpha_1 = 0, \alpha_3, \ldots, \alpha_n\}$. Now $\det(B_1)$ yielding $r_1 r_2 \cdots r_{\frac{n-1}{2}} = \alpha_2\alpha_4\cdots\alpha_{n-1}$ (the calculation is similar to the case of even n), where $\alpha_2, \alpha_4, \ldots, \alpha_{n-1}$ are the odd eigenvalues of L. The $(1,1)$ minor of B_2 is just $\det(B_1) = r_1 r_2 \cdots r_{\frac{n-1}{2}}$. Now we calculate the other principal minors of size $\frac{n-1}{2}$ of B_2. Fix such a minor. If we take the factor $\sqrt{2}$ from the first row and the first column, then the principal minor that we seek is twice the principal minor of size $\frac{n-1}{2}$ of a Laplacian matrix; by the weighted matrix tree theorem, that minor is equal to the (1,1) minor of the Laplacian, which is $\det(B_1)$. Therefore the corresponding principal minors of B_2 are given by $2\det(B_1) = 2r_1 \cdots r_{\frac{n-1}{2}}$. Again, from the fact that the sum of all of B_2's principal minors of size $\frac{n-1}{2}$ is equal to the $(\frac{n-1}{2})$-th elementary symmetric function of $\alpha_1, \alpha_3, \cdots, \alpha_n$, we find that $r_1 \cdots r_{\frac{n-1}{2}} + \frac{n-1}{2} 2r_1 \cdots r_{\frac{n-1}{2}} = nr_1 \cdots r_{\frac{n-1}{2}} = \alpha_3\alpha_5 \cdots \alpha_n$. Combining this equation with the one for B_1, we have $n\alpha_2\alpha_4 \cdots \alpha_{n-1} = \alpha_3\alpha_5 \cdots \alpha_n$. This is a contradiction, since the left side of the equation is an odd number, while the right side is an even number.

This completes the case of odd n. $\square$

4.3.2 One class of weighted mirror symmetric trees that do not have Laplacian PST between mirror symmetric vertices

We note that it was recently (in 2015) found [35] that there is no Laplacian PST for (unweighted) trees on $n \geq 3$ vertices. Theorem 4.3.1 resolves the weighted generalization for the special case of paths where PST between the end vertices is considered. In fact, we can generalize Theorem 4.3.1 to a class of weighted trees whose Laplacian matrix is persymmetric. Such a weighted tree, say Y, can be represented schematically as follows (see Figure 4.1):

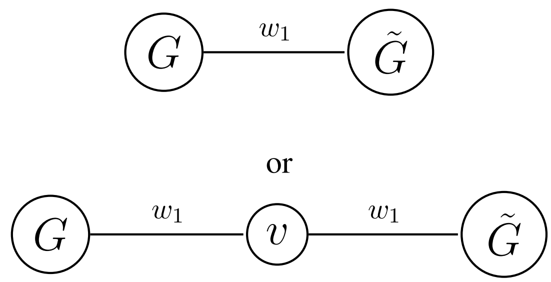


Figure 4.1: Symmetric trees

where G is a weighted tree, $\tilde{G}$ is the mirror image of G, and w_1 is an edge weight. Examples of weighted symmetric trees are shown in Figure 4.2.

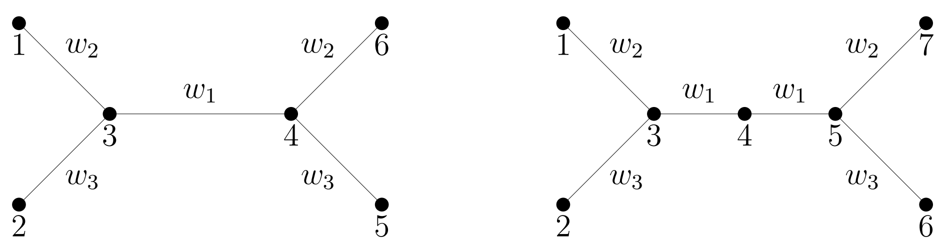


Figure 4.2: Weighted symmetric trees

The first graph (with a weighted edge connecting a vertex in G to its corresponding vertex in $\tilde{G}$) generalizes weighted paths on even number of vertices, and its Laplacian matrix is $L(Y) = \begin{bmatrix} E & RCR \\ C & RER \end{bmatrix}$, where $E = L(G) + w_1 e_{\frac{n}{2}} e_{\frac{n}{2}}^T$, C is of size $\frac{n}{2} \times \frac{n}{2}$, with its $(1, \frac{n}{2})$-entry equal to $-w_1$, and all the other entries zero. The second graph (with one middle vertex v connected to a vertex in G and to the corresponding vertex in $\tilde{G}$) generalizes weighted paths on odd number of vertices, and its Laplacian matrix is $L(Y) = \begin{bmatrix} E & x & 0 \\ x^T & 2w_1 & x^T R \\ 0 & Rx & RER \end{bmatrix}$, where $x = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ -w_1 \end{bmatrix} \in \mathbb{R}^{\frac{n-1}{2}}$, and $E = L(G) + w_1 e_{\frac{n-1}{2}} e^T_{\frac{n-1}{2}}$.

Theorem 4.3.2. *Let Y be a weighted mirror symmetric tree on n vertices as in Figure 4.1 (namely, a weighted tree whose Laplacian matrix is persymmetric). If n is even, let $B_1 = L(G) + 2w_1 e_{\frac{n}{2}} e^T_{\frac{n}{2}}$ and $B_2 = L(G)$. If n is odd, let $B_1 = L(G) + w_1 e_{\frac{n-1}{2}} e^T_{\frac{n-1}{2}}$ and $B_2 = \begin{bmatrix} 2w_1 & \sqrt{2}x^T \\ \sqrt{2}x & L(G) + w_1 e_{\frac{n-1}{2}} e^T_{\frac{n-1}{2}} \end{bmatrix}$. Suppose that B_1 and B_2 can be diagonalized by some real symmetric matrices Q_1 and Q_2, respectively, such that for some $j < \dfrac{n+1}{2}$, neither Q_1 nor Q_2 contains a zero entry in j-th row. Then the weighted mirror symmetric tree Y does not admit Laplacian PST between vertex j and its mirror image $n+1-j$. Therefore, if Q_1 contains no zero entries, and Q_2 contains no zero entries if n is even and contains no zero entries apart from the first row if n is odd, then the weighted tree Y does not admit Laplacian PST between any mirror symmetric vertex pairs.*

Proof. By a proper scaling of the Laplacian, we assume that PST occurs at time π. By Lemma 4.2.1, we know the Laplacian matrix $L(Y)$ is orthogonally similar to the block diagonal matrix $\begin{bmatrix} B_1 & 0 \\ 0 & B_2 \end{bmatrix}$, and therefore $\sigma(L(Y)) = \sigma(B_1) \cup \sigma(B_2)$.

Assume n is even. Observe that if v is an eigenvector of $B_1 = E - RC = L(G) + 2w_1 e_{\frac{n}{2}} e^T_{\frac{n}{2}}$ associated to the eigenvalue λ, i.e., $(E - RC)v = \lambda v$, then from $L(Y) \begin{bmatrix} v \\ -Rv \end{bmatrix} = \begin{bmatrix} E & RCR \\ C & RER \end{bmatrix} \begin{bmatrix} v \\ -Rv \end{bmatrix} = \begin{bmatrix} Ev - RCv \\ Cv - REv \end{bmatrix} = \lambda \begin{bmatrix} v \\ -Rv \end{bmatrix}$, we know that the antisymmetric vector $\begin{bmatrix} v \\ -Rv \end{bmatrix}$ is an eigenvector of the Laplacian matrix $L(Y)$ associated to the eigenvalue λ. Similarly, if u is the eigenvector of $B_2 = E + RC = L(G)$ associated to the eigenvalue μ, then the symmetric vector $\begin{bmatrix} u \\ Ru \end{bmatrix}$ is an eigenvector of $L(Y)$ associated to the eigenvalue μ. Using all the $n/2$ orthogonal eigenvectors v_k of B_1 and the $n/2$ orthogonal eigenvectors u_k of B_2, we can form n orthogonal eigenvectors of $L(Y)$: $\begin{bmatrix} v_k \\ -Rv_k \end{bmatrix}$, $\begin{bmatrix} u_k \\ Ru_k \end{bmatrix}$, $k = 1, \ldots, n/2$. Normalize each of them and use them as columns to form a real orthogonal matrix S. Then S diagonalizes $L(Y)$; assume that S diagonalizes $L(Y)$ to Λ. If there is PST between a vertex j and its mirror image $n+1-j$ at time π, then Proposition 2.6.2 implies that

$$s_j^T e^{i\pi\Lambda} = e^{i\phi} s_{n+1-j}^T, \tag{4.25}$$

where s_ℓ^T is the ℓ-th row of S and ϕ is some real number. From the fact that the eigenvector of $L(Y)$ associated to eigenvalue 0 is symmetric, we know that $e^{i\phi} = 1$. If S does not have any zero entries in its j-th row, then equation (4.25) implies that the symmetric eigenvectors of $L(Y)$ (constructed from the eigenvectors of B_2) are all associated to even eigenvalues, and the antisymmetric eigenvectors of $L(Y)$ (constructed from the eigenvectors of B_1) are all associated to odd eigenvalues. Therefore it follows that the eigenvalues of B_1 are odd integers and the eigenvalues of B_2 are even integers. Since $B_1 = B_2 + 2w_1 e_{\frac{n}{2}} e_{\frac{n}{2}}$, B_1 and B_2 are still rank-one perturbations of each other, and therefore their eigenvalues interlace. Now similar arguments as in Theorem 4.3.1 (if $n > 4$, we use the arguments in Theorem 4.3.1, and if $n = 4$, the graph is just a weighted path, and we use the conclusion of Theorem 4.3.1) imply that there is no Laplacian PST between the two mirror symmetric vertices j and $n+1-j$. Therefore, if Q_1 and Q_2 contain no nonzero entries, then Y does not admit Laplacian PST between any vertex and its mirror image.

If n is odd, then the Laplacian matrix of the weighted tree is $L(Y) = \begin{bmatrix} E & x & 0 \\ x^T & 2w_1 & x^T R \\ 0 & Rx & RER \end{bmatrix}$, where $x = \begin{bmatrix} 0 \cdots 0 & -w_1 \end{bmatrix}^T \in \mathbb{R}^{\frac{n-1}{2}}$. As above, we can check that if v is an eigenvector of $B_1 = E - RC = L(G) + w_1 e_{\frac{n-1}{2}} e_{\frac{n-1}{2}}^T$ associated to the eigenvalue λ, i.e., $B_1 v = \lambda v$, then $\begin{bmatrix} v \\ 0 \\ -Rv \end{bmatrix}$ is an eigenvector of $L(Y)$ associated to the eigenvalue λ. And if $u = \begin{bmatrix} a \\ \tilde{u} \end{bmatrix}$ is an eigenvector of $B_2 = \begin{bmatrix} 2w_1 & \sqrt{2}x^T \\ \sqrt{2}x & B_1 \end{bmatrix}$ associated to the eigenvalue μ, then $\begin{bmatrix} \tilde{u} \\ \sqrt{2}a \\ R\tilde{u} \end{bmatrix}$ is an eigenvector of $L(Y)$ associated to the eigenvalue μ. Using the $\frac{n-1}{2}$ eigenvectors v_k of B_1 and the $\frac{n+1}{2}$ eigenvectors u_ℓ of B_2, we form n orthogonal eigenvectors of $L(Y)$: $\begin{bmatrix} v_k \\ 0 \\ -Rv_k \end{bmatrix}$, $\begin{bmatrix} \tilde{u}_\ell \\ \sqrt{2}a \\ R\tilde{u}_\ell \end{bmatrix}$ for $k = 1, \ldots, \frac{n-1}{2}, \ell = 1, \ldots, \frac{n+1}{2}$. If Q_1 and Q_2 do not have any zero entries in the j-th row for some $j < \frac{n+1}{2}$, then with a similar argument as in the even case, we can see that if there is PST between the vertex j and its mirror image $n + 1 - j$, then the eigenvalues of B_1 are odd integers, and the eigenvalues of B_2 are even integers. Since B_2 is a bordered matrix of B_1, their eigenvalues interlace, and the arguments in Theorem 4.3.1 apply here. $\square$

Note that Theorem 4.3.2 implies Theorem 4.3.1, as the Laplacian matrix L of a weighted path on n vertices is diagonalizable by a real orthogonal matrix $Q = [a_k \tilde{p}_j(\alpha_k)]$, where the polynomials $\tilde{p}_j(x)$, $j = 0, \ldots, n$ form the sequence of orthogonal polynomials associated to the tridiagonal matrix L, the α_ks are the eigenvalues of L (roots of $p_n(x)$), and that each a_k is a nonzero constant scalar for a fixed k. Since each entry $a_k \tilde{p}_0(\alpha_k) = a_k$ in the first row of Q is nonzero, and the columns of Q are symmetric or antisymmetric eigenvectors of L (by Lemma 2.6.3, if a weighted path with loops admits PST between the end vertices, then it is mirror symmetric), Theorem 4.3.2 implies that there is no Laplacian PST between the end vertices of a weighted path.

Symmetric trees are a special case of graphs with an involution; the PST and PGST properties of such graphs were studied [64] under adjacency dynamics. The system considered by Kempton, Lippner and Yau [64] was with potentials (loops), and the results obtained are independent from the results of this section in a sense that neither implies the other.

4.4 Adjacency dynamics and a rational weights conjecture

For the rest of this chapter we focus on adjacency dynamics, giving a complete analysis of the 4×4 and 5×5 cases, and proving a more general result motivated by an observation made in these cases.

Example 4.4.1. For a weighted mirror-symmetric path (with no loops) on 4 vertices, write the eigenvalues $\alpha_1, \ldots, \alpha_4$ of the adjacency matrix A as $-\beta_2, -\beta_1, \beta_1, \beta_2$; then $r_2 = \frac{S_1}{2} = \beta_2 - \beta_1$. The fact that the product of all the eigenvalues of A equals the determinant of A

yields $r_1^4 = \det(A) = \beta_1^2\beta_2^2$, and therefore $r_1 = \sqrt{\beta_1\beta_2}$. The Hamiltonian is then

$$A = \begin{bmatrix} 0 & \sqrt{\beta_1\beta_2} & 0 & 0 \\ \sqrt{\beta_1\beta_2} & 0 & \beta_2-\beta_1 & 0 \\ 0 & \beta_2-\beta_1 & 0 & \sqrt{\beta_1\beta_2} \\ 0 & 0 & \sqrt{\beta_1\beta_2} & 0 \end{bmatrix}. \tag{4.26}$$

By Remark 4.1.9, the system with Hamiltonian A as in (4.26) admits PST at time π if and only if $2\beta_1 \equiv 1 \pmod 4$ and $2\beta_2 \equiv 3 \pmod 4$ or vice versa. It follows that $r_2 = \beta_2 - \beta_1$ is an odd integer. However, $4\beta_1\beta_2 \equiv 3 \pmod 4$, so the quantity is not a perfect square, and therefore $r_1 = \sqrt{\beta_1\beta_2}$ is irrational. There is no nonzero constant κ for which both $\kappa(\beta_2 - \beta_1)$ and $\kappa\sqrt{\beta_1\beta_2}$ are rational (κA has PST at time $\frac{1}{\kappa}\pi$). Therefore no weighted path without loops on four vertices with all weights being rational can have adjacency PST between the end vertices. In particular, the unweighted path P_4 does not admit adjacency PST. This observation motivates a more general result which we will present after the analysis of the 5×5 case.

Example 4.4.2 (5×5 Case)**.** For $n = 5$, we consider weighted mirror-symmetric paths without loops. The eigenvalues of the adjacency matrix A in this case are $-\beta_2 < -\beta_1 < \beta_0 = 0 < \beta_1 < \beta_2$, and the characteristic polynomial of A, expressed in terms of the eigenvalues, is $p_5(x) = x(x^2 - \beta_2^2)(x^2 - \beta_1^2)$, while direct computation shows that the characteristic polynomial of A, expressed in terms of the edge weights (i.e., entries of A), is $x(x^2 - r_1^2)(x^2 - (r_1^2 + 2r_2^2))$. Therefore $\beta_1 = r_1$, $\beta_2 = \sqrt{r_1^2 + 2r_2^2}$, as $\beta_1 < \beta_2$. Solving these two equations, we obtain $r_2^2 = \frac{\beta_2^2 - \beta_1^2}{2}$ (in fact we can get r_2 directly from

Proposition 4.2.2). The Hamiltonian is now

$$A = \begin{bmatrix} 0 & \beta_1 & 0 & 0 & 0 \\ \beta_1 & 0 & \sqrt{\frac{\beta_2^2-\beta_1^2}{2}} & 0 & 0 \\ 0 & \sqrt{\frac{\beta_2^2-\beta_1^2}{2}} & 0 & \sqrt{\frac{\beta_2^2-\beta_1^2}{2}} & 0 \\ 0 & 0 & \sqrt{\frac{\beta_2^2-\beta_1^2}{2}} & 0 & \beta_1 \\ 0 & 0 & 0 & \beta_1 & 0 \end{bmatrix}. \tag{4.27}$$

By Remark 4.1.9, a weighted path with adjacency matrix A as in (4.27) admits PST between end vertices at time π if and only if β_1 is an odd integer, and β_2 is an even integer. This gives us a lot of choices for the edge weight set $\{r_1, r_2\}$ of a weighted path on 5 vertices to allow adjacency PST (apart from the $\sqrt{j(n-j)}$ ones). As in $n = 4$ case, the parity of the two integers β_1 and β_2 implies that $r_1 = \beta_1 \in \mathbb{Z} \subseteq \mathbb{Q}$, and $r_2 = \sqrt{\frac{\beta_2^2-\beta_1^2}{2}} \notin \mathbb{Q}$. Hence no weighted path without loops on five vertices with all weights rational admits adjacency PST between the end vertices, in particular, the unweighted path P_5 does not admit adjacency PST.

Remark 4.4.3. The weighted path on n vertices with edge weights $\{w_{j,j+1} = \sqrt{j(n-j)} | j = 1, \ldots, n-1\}$ admits adjacency PST between its end vertices [30]. As shown in Example 4.4.1 and Example 4.4.2, by choosing proper integers or half integers, we can obtain many other edge weights set for a weighted path on four or five vertices to exhibit adjacency PST between the end vertices.

Theorem 4.3.1 tells us that no weighted path of length at least 3 has Laplacian PST between its end vertices; however there is a weighted path (with no loops) of any length that admits adjacency PST between its end vertices [30]. Here we make a conjecture about the weights: if all the weights of a weighted path on at least 4 vertices are rational numbers, then there is no adjacency PST at time π between the end vertices of the path. We confirm that conjecture in the cases $n = 4$, $n \equiv 3 \pmod 8$ and $n \equiv 5 \pmod 8$.

Proposition 4.4.4. *Suppose that* $n = 4$, *or* $n \equiv 3 \pmod 8$ *or* $n \equiv 5 \pmod 8$. *If the weights of a weighted path on* n *vertices with or without potentials are all rational numbers, then there is no adjacency PST between its end vertices at readout time* π.

Proof. As discussed in Remark 4.1.10, if a weighted path exhibits PST at time π between its end vertices, then by performing an overall energy shift if necessary (which does not change the PST time), we can make all its eigenvalues integers (in particular, with the smallest one being an odd integer). Then the ordered eigenvalues are of alternating parity.

For $n = 3$, we know that the weighted path with loops on three vertices with eigenvalues $\alpha_1, \alpha_2, \alpha_3$ has adjacency matrix A as in (4.18), in particular, $r_1 = \frac{\sqrt{-2\alpha_2^2+2\alpha_1\alpha_2-2\alpha_1\alpha_3+2\alpha_2\alpha_3}}{2} = \frac{\sqrt{2(\alpha_3-\alpha_2)(\alpha_2-\alpha_1)}}{2} \notin \mathbb{Q}$, as α_1, α_3 are odd, and α_2 is even for A to admit PST at time π.

For $n = 4$, we know the adjacency matrix $A = \begin{bmatrix} q_1 & r_1 & 0 & 0 \\ r_1 & q_2 & r_2 & 0 \\ 0 & r_2 & q_2 & r_1 \\ 0 & 0 & r_1 & q_1 \end{bmatrix}$ is similar to $\begin{bmatrix} B_1 & O \\ O & B_2 \end{bmatrix}$, with $B_1 = \begin{bmatrix} q_1 & r_1 \\ r_1 & q_2 - r_2 \end{bmatrix}$, $B_2 = \begin{bmatrix} q_1 & r_1 \\ r_1 & q_2 + r_2 \end{bmatrix}$. As in the proof of Proposition 4.2.2, the eigenvalues of B_1 are odd integers α_1 and α_3, and the eigenvalues of B_2 are even integers α_2 and α_4. In addition, Proposition 4.2.2 says that $r_2 = \frac{S_1}{2} \in \mathbb{Q}$ and $q_2 = \frac{S_2}{2S_1}$. Now

$$\det(B_1) = q_1(q_2 - r_2) - r_1^2 \quad = \quad \alpha_1\alpha_3 \tag{4.28}$$

$$\det(B_2) = q_1(q_2 + r_2) - r_1^2 \quad = \quad \alpha_2\alpha_4 \tag{4.29}$$

Subtracting (4.28) from (4.29) yields $q_1 = \frac{\alpha_2\alpha_4 - \alpha_1\alpha_3}{2r_2} = \frac{\alpha_2\alpha_4 - \alpha_1\alpha_3}{S_1}$. Substituting q_1, q_2 and r_2 back to (4.28) gives that $r_1 = \sqrt{\frac{(\alpha_2\alpha_4 - \alpha_1\alpha_3)S_2 - (\alpha_2\alpha_4 + \alpha_1\alpha_3)S_1^2}{2S_1^2}}$. We now show that r_1 is irrational by showing that $r_1^2 S_1^2 = \frac{(\alpha_2\alpha_4 - \alpha_1\alpha_3)S_2 - (\alpha_2\alpha_4 + \alpha_1\alpha_3)S_1^2}{2}$ is not a perfect square (as $S_1 \in \mathbb{Z}$). Rearranging the terms gives

$$\begin{aligned}
&\frac{1}{2}(\alpha_2\alpha_4(S_2 - S_1^2) - \alpha_1\alpha_3(S_2 + S_1^2)) \\
&\quad = -\alpha_2\alpha_4(\alpha_1^2 + \alpha_3^2) - \alpha_1\alpha_3(\alpha_2^2 + \alpha_4^2) + \\
&\quad \alpha_2\alpha_4 \times (\alpha_1\alpha_2 - \alpha_1\alpha_3 + \alpha_1\alpha_4 + \alpha_2\alpha_3 - \alpha_2\alpha_4 + \alpha_3\alpha_4) \\
&\quad - \alpha_1\alpha_3\alpha_2\alpha_4 + \alpha_1\alpha_3(\alpha_1 + \alpha_3)(\alpha_2 + \alpha_4) - \alpha_1^2\alpha_3^2.
\end{aligned} \tag{4.30}$$

From the fact that α_1 and α_3 are odd integers, and α_2 and α_4 are even integers, we know that the first 5 terms in the summand are all divisible by 4, and therefore their sum is congruent to $0 \pmod 4$. Since the square $\alpha_1^2\alpha_3^2$ of the odd integer $\alpha_1\alpha_3$ is congruent to $1 \pmod 8$ (therefore also $1 \pmod 4$), it follows that the result in equation (4.30) is congruent to $3 \pmod 4$, and hence is not a perfect square. Thus r_1 is not rational (while r_2 is), which establishes the result for $n = 4$. In fact as mentioned in Example 4.4.1, we can say more in this case: if the weights of a weighted path on 4 vertices are all rational numbers, then the weighted path does not admit adjacency PST between its end vertices at any time (not just π).

Next, suppose that $n \geq 5$ and $n \equiv 3 \pmod 8$ or $n \equiv 5 \pmod 8$. Observe that since n is odd, Proposition 4.2.2 implies that $r_{\frac{n-1}{2}} = \dfrac{\sqrt{S_2 - S_1^2}}{2}$. We claim now that the quantity $S_2 - S_1^2$ is not a perfect square, and so $r_{\frac{n-1}{2}}$ is irrational. To see this, note that $S_2 - S_1^2 = -2[\sum_r \alpha_{2r}^2 + \sum_{1 \leq j < k \leq n} (-1)^{j+k} \alpha_j \alpha_k]$, where $\sum_r \alpha_{2r}^2$ is divisible by 4.

Consequently, $2\sum_r \alpha_{2r}^2 \equiv 0 \pmod 8$.

If we show that $\sum_{1\leq j<k\leq n}(-1)^{j+k}\alpha_j\alpha_k$ is odd, then we can conclude that $S_2 - S_1^2$ is not a perfect square. To this end, it is enough to count the number of distinct pairs of odd numbers appearing in the summation. Write n as $n = 2m-1$ for some $m \in \mathbb{Z}$. Then there are m odd integers in the set $\{1,\ldots,n\}$, and the number of distinct odd pairs is $m(m-1)/2$. For $n \equiv 3 \pmod 8$ or $n \equiv 5 \pmod 8$, we have $m \equiv 2 \pmod 4$ or $m \equiv 3 \pmod 4$, respectively. In either case, $m(m-1)/2$ is odd and the claim follows. Thus $S_2 - S_1^2$ is not a perfect square, so $r_{\frac{n-1}{2}}$ is not rational.

$\square$

Chapter 5

Switching and partially switching the hypercube while maintaining perfect state transfer

The n-cube has a lot of nice properties: it is diagonalizable by the standard Hadamard matrix, with all the eigenvalues being even integers, has Laplacian and adjacency PST at time $\pi/2$ between any pair of antipodal vertices (for each vertex of the n-cube, there is exactly one vertex at distance n from it, and they are said to be antipodal to each other). The hypercubes form a family of highly structured graphs that exhibit PST. As discussed in Section 3.3, there are connected d-regular (n-cubelike) graphs on 2^n vertices that are diagonalizable by the standard Hadamard matrix H_n and exhibit PST for any $d \in \{n, \ldots, 2^n - 1\}$, with the PST distance (distance between the sender vertex and the receiver vertex) less than or equal to n (with equality for the n-cube), but these graphs are more sensitive to timing errors than the hypercube by Theorem 2.6.4.

One is often interested in sending the state as far as possible along the spin network (maximizing the PST distance), and ensuring that the state transfer is as insensitive as possible to errors in the readout time (that is, if a graph exhibits PST at time $t = t_0$, then one would hope the graph to exhibit near-perfect state transfer at time $t = t_0 \pm \epsilon$, for small ϵ). Therefore an n-cubelike graph with fewer edges has better PST properties (less sensitive to readout errors, by Theorem 2.6.4). We will see in Section 5.1, that deleting edges in the n-cube does not result in connected graphs that are diagonalizable by the standard Hadamard matrix H_n; this leads us to consider n-regular graphs that can be obtained from the n-cube by adding and deleting edges. The switched n-cube is one such graph. Although it turns out not to be Hadamard diagonalizable (see Theorem 5.2.5), it indeed shares many of the same properties as the n-cube: it is cospectral to the n-cube (they have the same set of eigenvalues, counting multiplicity), it is n-regular, it exhibits PST at time $\pi/2$, its PST distance is n, and it has the same sensitivity as the n-cube to timing errors when PST occurs.

Godsil-McKay (GM) switching [48] is a graph operation that perturbs a graph by removing and creating edges based on certain criteria that a partition of the vertex set must satisfy (see Section 2.3.2 for more precise details); the resulting graph is cospectral to the original graph but is often non-isomorphic to the original graph. We apply GM switching to the hypercube as a means of constructing non-isomorphic graphs that have many of the same properties of the hypercube, including PST.

In Section 5.1, we give an inductive proof of the fact that no connected proper spanning subgraphs of the n-cube are diagonalizable by the standard Hadamard matrix, without using the fact that a graph is diagonalizable by a standard Hadamard matrix if and only if it is a cubelike graph. In Section 5.2, we use Godsil-McKay switching to construct a graph (the switched n-cube) of order 2^n for $n > 4$ that has many of the same properties as the n-cube (in particular, it admits PST between certain pair of vertices that exhibits PST in the n-cube), but is nevertheless non-isomorphic to the n-cube, and is not Hadamard-diagonalizable. In Section 5.3, we then consider partially switched n-cubes, which generalize the process of GM switching on the n-cube by considering it as the Cartesian product of the $(n-4)$-cube with the 4-cube, and performing GM switching on some copies of the 4-cube. These new graphs are not cospectral to the n-cube in general, but do exhibit PST (though in significantly fewer pairs of vertices). In Section 5.4, we further generalize this by replacing each copy of the 4-cube by a convex combination of the 4-cube and the switched 4-cube; we also generalize it to a time-dependent Hamiltonian (see, e.g. [79]) that alternates between the various graphs considered. We give motivation as to why these families of graphs might be useful in practice; in particular, we conduct a sensitivity analysis with respect to readout time errors in Section 5.5.

We state the results in terms of the adjacency matrix. Again, as mentioned in Proposition 1.3.10, since the graphs we discuss in this chapter are regular, most of the results hold for the Laplacian matrix. Throughout this chapter, we use I_m to denote the identity matrix of size m, $I_{(m)}$ to denote the identity matrix of size 2^m, J_m to denote the all-ones matrix of size $m \times m$, $J_{(m)}$ to denote the all-ones matrix of size $2^m \times 2^m$, $\mathbf{1}_m$ to denote the all-ones vector of length m, and $\mathbf{1}_{(m)}$ to denote the all-ones vector of length 2^m. This chapter is based on work with Kirkland and Plosker [68], with myself as primary author.

5.1 No connected proper spanning subgraphs of hypercubes are diagonalizable by the standard Hadamard matrix

By making use of the result that a graph is diagonalizable by the standard Hadamard matrix if and only if it is a cubelike graph (Corollary 3.6.2), we could prove that deleting edges in hypercubes (while keeping all the vertices) will not result in connected graphs that are still diagonalizable by the standard Hadamard matrix. In fact, as a special Cayley graph, we know that a cubelike graph is connected if and only if its connection set C contains a basis of $\mathbb{Z}_2^n$, viewed as a vector space (Theorem 2.5.3). Since $\mathbb{Z}_2^n$ is n-dimensional, we know that a connected n-cubelike graph is regular with degree at least n. Therefore for any positive integer n, no connected graphs on 2^n vertices that have fewer edges than the n-cube are diagonalizable by the standard Hadamard matrix H_n. So we cannot perturb the hypercube by deleting edges, without adding edges as well, while still maintaining PST, connectivity, and diagonalizability by the standard Hadamard matrix. The switched cube discussed in Section 5.2 maintains the same sparsity structure (the same number of edges) as the n-cube, some PST pairs (though not all), but is not Hadamard diagonalizable anymore.

Here, without appealing to cubelike graphs, we give an alternate proof of the fact that removing at least one edge from the n-cube cannot produce a connected graph that is diagonalizable by the standard Hadamard matrix H_n.

Proposition 5.1.1. *No connected proper spanning subgraphs of hypercubes are diagonalizable by the standard Hadamard matrix H_n.*

Proof. Let C_n denote the adjacency matrix of Q_n. We prove by induction on n that any subgraph of Q_n that is diagonalizable by H_n is not connected.

If $n = 1$, there are no connected proper spanning subgraphs of the 1-cube, and hence the result holds. Assume the statement is true for $n = k - 1$, and we show that it is true for $n = k$. If we consider the k-cube as the Cartesian product of K_2 with the $(k-1)$-cube, we know $C_k = \begin{bmatrix} C_{k-1} & I_{(k-1)} \\ I_{(k-1)} & C_{k-1} \end{bmatrix}$. Let Y be any proper spanning subgraph of Q_k that is diagonalizable by H_k; denote its adjacency matrix by M . Then $M = \begin{bmatrix} M_1 & D \\ D & M_2 \end{bmatrix}$, where D is a diagonal matrix with the diagonal entries being either 0 or 1, and M_1, M_2 are both (symmetric) adjacency matrices of some subgraphs of the $(k-1)$-cube. Now

$$2^k H_k^{-1} M H_k = H_k^T M H_k = \begin{bmatrix} H_{k-1}^T & H_{k-1}^T \\ H_{k-1}^T & -H_{k-1}^T \end{bmatrix} \begin{bmatrix} M_1 & D \\ D & M_2 \end{bmatrix} \begin{bmatrix} H_{k-1} & H_{k-1} \\ H_{k-1} & -H_{k-1} \end{bmatrix}$$

$$= \begin{bmatrix} H_{k-1}^T M_1 H_{k-1} + H_{k-1}^T M_2 H_{k-1} + 2H_{k-1}^T D H_{k-1} & H_{k-1}^T M_1 H_{k-1} - H_{k-1}^T M_2 H_{k-1} \\ H_{k-1}^T M_1 H_{k-1} - H_{k-1}^T M_2 H_{k-1} & H_{k-1}^T M_1 H_{k-1} + H_{k-1}^T M_2 H_{k-1} - 2H_{k-1}^T D H_{k-1} \end{bmatrix}$$

is diagonal. So $H_{k-1}^T M_1 H_{k-1} = H_{k-1}^T M_2 H_{k-1}$, which implies that $M_1 = M_2$. Therefore we can assume $M = \begin{bmatrix} M_1 & D \\ D & M_1 \end{bmatrix}$, and hence the equation $2^k H_k^{-1} M H_k = H_k^T M H_k$ above simplifies to $\begin{bmatrix} 2H_{k-1}^T M_1 H_{k-1} + 2H_{k-1}^T D H_{k-1} & 0 \\ 0 & 2H_{k-1}^T M_1 H_{k-1} - 2H_{k-1}^T D H_{k-1} \end{bmatrix}$. Again from the fact that the above matrix is diagonal, we know the matrices $2H_{k-1}^T M_1 H_{k-1} + 2H_{k-1}^T D H_{k-1}$ and $2H_{k-1}^T M_1 H_{k-1} - 2H_{k-1}^T D H_{k-1}$ are both diagonal, therefore $H_{k-1}^T M_1 H_{k-1}$ is diagonal. By the induction assumption, the subgraph G_1 with adjacency matrix M_1 of Q_{k-1} is not connected, therefore neither is Y (which is $K_2 \square G_1$ with possibly some edges between the two copies of G_1 removed).

$\square$

5.2 A graph cospectral to the n-cube with PST

In this section, we give a cospectal mate of the n-cube that is no longer Hadamard diagonalizable, but is n-regular, exhibits PST, and has PST distance n. We will make use of Godsil-McKay (GM) switching (see Section 2.3.2).

5.2.1 The switched n-cube

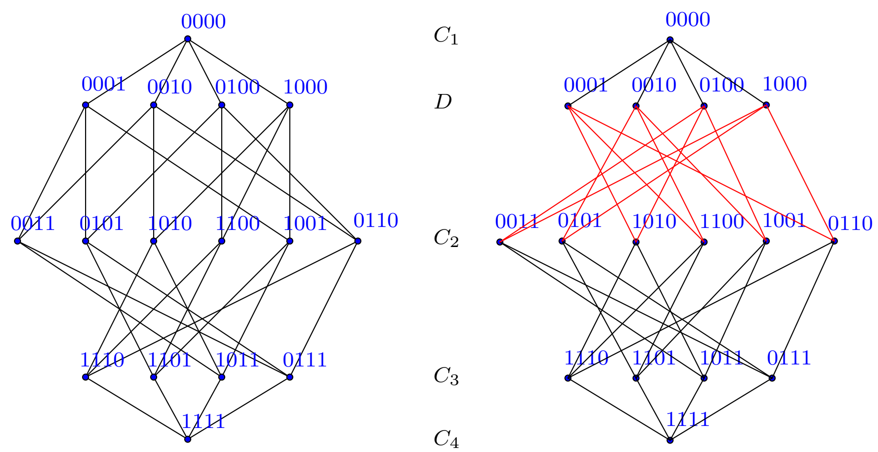
In [19, Section 1.8], a cospectral mate of the 4-cube is given; this graph and the 4-cube are both bipartite, with partition where one of the two parts being

$$
\begin{aligned}
C &= \{0000, 0011, 0101, 0110, 1001, 1010, 1100, 1111\} \quad \text{(for the 4-cube) or} \\
C' &= \{0000, 0011, 0101, 0110, 1000, 1011, 1101, 1110\} \quad \text{(for the cospectral mate),}
\end{aligned}
$$

and the other class of the vertex set consists of vertices with labels (a, b), where $a \in \{1, 2, 3, 4\}$ indicates the digit position (here we start counting from the right) and $b \in \{0, 1\}$ indicates the binary value at this position. For example, vertex 0101 is adjacent to (1,1), (2,0), (3,1) and (4,0). The two graphs can be obtained from each other by GM switching with respect to the neighbourhood of one vertex [19].

Now we show it in detail by using the usual labelling of the 4-cube Q_4: binary strings of length 4 (Section 2.5.1). Partition the vertex set $V(Q_4)$ in the following way: vertex 0000 forms C_1; vertices that are at distance 2 from vertex 0000 (which are 0011, 0101, 1010, 1100, 1001, and 0110) form C_2; vertices that are at distance 3 from vertex 0000 (which are 1110, 1101, 1011, and 0111) form C_3; vertex 1111, the only vertex at distance 4 from 0000, forms C_4; vertices that are at distance 1 from vertex 0000 (which are 0001, 0010, 0100, and 1000) form D (i.e., this partition is in fact the distance partition with respect to vertex 0000). Then this partition π satisfies the conditions for GM switching, and $Q_4^{(\pi)}$ — the local switching of Q_4 with respect to π, is the above cospectral mate of Q_4, as Figure 5.1 shows. We call $Q_4^{(\pi)}$ the *switched 4-cube* and denote it as $\tilde{Q}_4$. We order the vertices of Q_4 and $\tilde{Q}_4$ (from 1 to 16) according to the partition, in the order C_1, D, C_2, C_3, C_4, and in each cell we order the vertices in the increasing lexicographic order of the binary representations of vertices. Therefore, from top to bottom, and from left to right, the vertices in Figure 5.1 are 1, 2, 3, 4, 5, 6, 7, 10, 11, 9, 8, 15, 14, 13, 12 and 16 (the adjacency matrix of the switched 4-cube is shown in Lemma 5.2.4 below).

Consider the following recursive way to construct the n-cube Q_n: take two disjoint



4-cube Q_4 Switched 4-cube $\tilde{Q}_4 = Q_4^{(\pi)}$

Figure 5.1: Order the vertices of Q_4 and $\tilde{Q}_4$ so that the order from top to bottom and from left to right is 1, 2, 3, 4, 5, 6, 7, 10, 11, 9, 8, 15, 14, 13, 12 and 16

copies of the $(n-1)$-cube, then connect the corresponding vertices in the two copies to obtain the n-cube ($Q_n = K_2 \square Q_{n-1}$). Starting with the above 4-cube, we now consider the 5-cube $Q_5 = K_2 \square Q_4$. Partition the vertex set of each of the two copies of the 4-cube in the above way, i.e., the distance partition on the two induced subgraphs Q_4 in Q_5; note that they form a partition, say π_1, of the vertex set of the 5-cube, and it is an equitable partition. If we take the union of the two D cells (i.e., the vertices at the second level in height starting from the top, as shown in Figure 5.2) of the partition of each copy of Q_4 to form a larger partition cell and keep all the other cells unchanged, we can see that the new partition π_2 of the vertex set of the 5-cube satisfies the GM switching conditions, and the local switching of Q_5 with respect to π_2 — the switched 5-cube is shown in Figure 5.3.

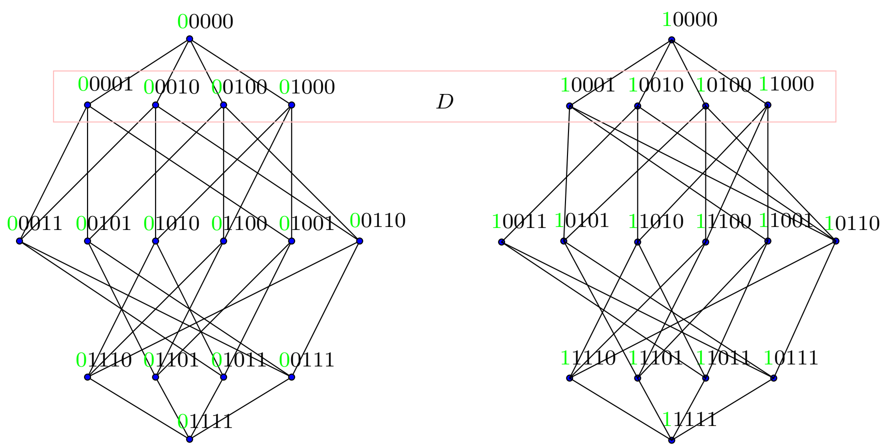


Figure 5.2: Applying GM switching to the 5-cube. Note that the edges between the corresponding vertices in the two copies of the 4-cube are omitted.

In general, consider two different partitions of the vertex set of $Q_n = Q_{n-4}\Box Q_4$. We partition the vertex set of each of the 2^{n-4} copies of the 4-cube according to π as shown in Figure 5.1, then the cells $C_1^{(j)}, D^{(j)}, C_2^{(j)}, C_3^{(j)}, C_4^{(j)}$, $j = 1, \ldots 2^{n-4}$ form a partition of the vertex set of Q_n, where $C_1^{(j)}, D^{(j)}, C_2^{(j)}, C_3^{(j)}, C_4^{(j)}$ is the distance partition of the vertex set of j-th copy of the 4-cube as shown in Figure 5.1. We denote this partition by π_1; it is an equitable partition of Q_n. Now, we take the union of all the 2^{n-4} $D^{(j)}$ cells to form a new larger cell $D_0 = D^{(1)} \cup \cdots \cup D^{(2^{n-4})}$. Then the new partition $D_0, C_1^{(j)}, C_2^{(j)}, C_3^{(j)}, C_4^{(j)}$, $j = 1, \ldots 2^{n-4}$ of $V(Q_n)$ satisfies the GM switching conditions, and we denote this partition by π_2.

Remark 5.2.1. Note that for the switched n-cube or a partially switched n-cube that are

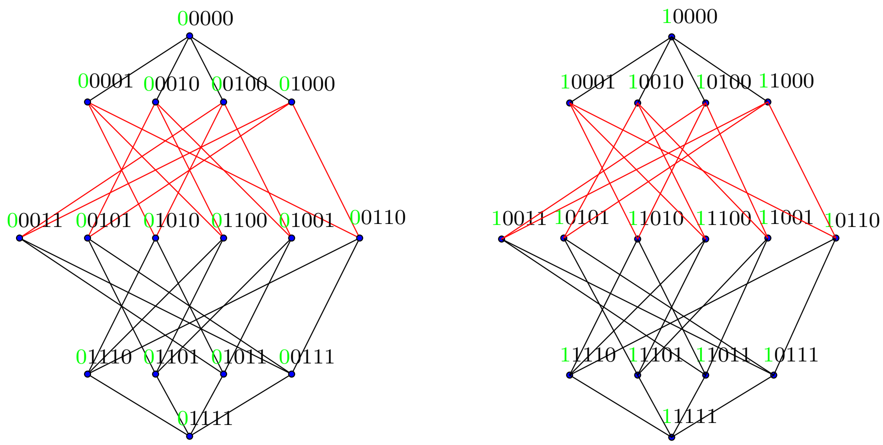


Figure 5.3: The switched 5-cube with edges between corresponding vertices between the two copies of the switched 4-cube omitted.

discussed in the later part of this chapter, π_1 is still equitable and π_2 still satisfies the GM switching conditions.

Using the partition π_2 of $V(Q_n)$ and applying the GM switching, we can get a cospectral mate — the switched cube of the n-cube — for each $n \geq 4$. Denote the switched n-cube $Q_n^{(\pi)}$ by $\tilde{Q}_n$, the adjacency matrix of Q_n by C_n, and the adjacency matrix of $\tilde{Q}_n$ by $\tilde{C}_n$.

Investigating the construction, we see that $\tilde{Q}_n$ is the Cartesian product of Q_{n-4} with $\tilde{Q}_4$ for $n > 4$. For the n-cube $Q_n = Q_{n-4} \Box Q_4$, or the switched n-cube $\tilde{Q}_n = Q_{n-4} \Box \tilde{Q}_4$, we order the vertices of Q_4 or $\tilde{Q}_4$ as in Figure 5.1, order the vertices of Q_{n-4} in the increasing lexicographic order of their binary representation, and finally order the vertices of the Cartesian products in accordance with the lexicographic ordering, that is, $A(Q_n) = A(Q_{n-4}) \otimes I_{(4)} + I_{(n-4)} \otimes A(Q_4)$ and $A(\tilde{Q}_n) = A(Q_{n-4}) \otimes I_{(4)} + I_{(n-4)} \otimes A(\tilde{Q}_4)$ (Theorem 2.2.5). In the following, when we say replace some copy of Q_4 inside Q_n by $\tilde{Q}_4$, $\tilde{Q}_4$ is always obtained from Q_4 by GM switching with respect to π as in Figure 5.1, i.e., the distance partition of that 4-cube with respect to vertex $x0000$, where $x \in \mathbb{Z}_2^{n-4}$ indicates which copy this 4-cube is (inside the n-cube).

The non-isomorphism of $\tilde{Q}_n$ and Q_n can be seen directly from the fact that they exhibit different PST properties: namely, they have different numbers of PST vertex pairs, as we will see in the next section.

5.2.2 PST property and non-Hadamard diagonalizablity of the switched n-cube

Theorem 5.2.2. *For $n \geq 4$, exactly half of the vertices of the switched n-cube $\tilde{Q}_n$ pair up to have PST between each other at time $\pi/2$.*

Proof. Since the eigendecomposition of $\tilde{C}_4$ ($\tilde{C}_4$ is diagonalizable by QH_4, where Q is the similarity matrix between C_4 and $\tilde{C}_4$ as mentioned in Section 2.3.2) is known in closed form, we may explicitly compute $e^{i\tilde{C}_4\pi/2}$, also in closed form. From that explicit computation, we can see that there is PST between vertices 1 and 16, 6 and 11, 7 and 10, 8 and 9 in $\tilde{Q}_4$ at time $\pi/2$ (whereas Q_4 admits PST between vertices j and $17 - j$ for each j); exactly half (8 out of 16) of the vertices pair up in $\tilde{Q}_4$ to exhibit PST. Recall that the adjacency matrix of $\tilde{Q}_n$ is $\tilde{C}_n = C_{n-4} \otimes I_{(4)} + I_{(n-4)} \otimes \tilde{C}_4$. Therefore

$$\begin{aligned} U_{\tilde{Q}_n}(\pi/2) &= e^{i(\pi/2)\tilde{C}_n} = e^{i(\pi/2)(C_{n-4}\otimes I_{(4)}+I_{(n-4)}\otimes\tilde{C}_4)} \\ &= e^{i(\pi/2)C_{n-4}\otimes I_{(4)}} e^{i(\pi/2)I_{(n-4)}\otimes\tilde{C}_4} = e^{i(\pi/2)C_{n-4}} \otimes e^{i(\pi/2)\tilde{C}_4} \\ &= i^{(n-4)} \begin{bmatrix} 0 & 0 & \cdots & 0 & e^{i(\pi/2)\tilde{C}_4} \\ 0 & 0 & \cdots & e^{i(\pi/2)\tilde{C}_4} & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & e^{i(\pi/2)\tilde{C}_4} & \cdots & 0 & 0 \\ e^{i(\pi/2)\tilde{C}_4} & 0 & \cdots & 0 & 0 \end{bmatrix}, \end{aligned}$$

where the third equation is based on the fact that $C_{n-4} \otimes I_{(4)}$ and $I_{(n-4)} \otimes \tilde{C}_4$ commute. Since half of the rows of $e^{i(\pi/2)\tilde{C}_4}$ have an (off-diagonal) entry with modulus 1 and none of the diagonal entry have modulus 1, then so is $e^{i(\pi/2)\tilde{C}_n}$, i.e., half of the vertices of $\tilde{Q}_n$ pair up to have PST between each other at time $\pi/2$. □

From the proof of Theorem 5.2.2, it can be checked that in the labeling of vertices as described at the end of Section 5.2.1, PST in $\tilde{Q}_n$ is between vertex $j + 2^4m_4 + 2^5m_5 + \cdots + 2^{n-1}m_{n-1}$ and $17 - j + 2^4(1 - m_4) + 2^5(1 - m_5) + \cdots + 2^{n-1}(1 - m_{n-1})$, where $m_k \in \{0, 1\}$ for $k = 4, \ldots, n-1$ and $j = 1, 6, 7, 8, 9, 10, 11, 16$, and PST in Q_n is between ℓ and $2^n + 1 - \ell$ for each ℓ. We thus make the following remark, implying that the two graphs Q_n and $\tilde{Q}_n$ are non-isomorphic.

Remark 5.2.3. There are half as many vertex pairs for which PST occurs (at time $\pi/2$) in the switched n-cube as there are in the n-cube, and the PST pairs of the switched n-cube form a subset of the PST pairs of the n-cube.

The following Hadamard diagonalizable property gives an alternate proof of the fact that $\tilde{Q}_n$ is not isomorphic to Q_n for $n \geq 4$. As a direct consequence, the switched n-cube is not Hadamard diagonalizable.

Lemma 5.2.4. *The adjacency matrix of the switched 4-cube $\tilde{Q}_4$ does not have a $(1,-1)$-eigenvector associated to eigenvalue 2.*

Proof. The adjacency matrix $\tilde{C}_4$ of $\tilde{Q}_4$ (with vertices labelled and ordered as in Figure 5.1) is

$$\tilde{C}_4 = \begin{bmatrix}
0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0
\end{bmatrix}.$$

The reduced row echelon form R of $\tilde{C}_4 - 2I_{(4)}$ is

$$R = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & -1 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & 0 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & -2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}.$$

Thus we get four linearly independent eigenvectors associated to 2:

$$\begin{aligned} v_1 &= [0,0,0,-1,1,0,1,1,-1,-1,0,1,-1,0,0,0]^T, \\ v_2 &= [0,0,-1,0,1,1,0,1,-1,0,-1,1,0,-1,0,0]^T, \\ v_3 &= [0,-1,0,0,1,1,1,0,0,-1,-1,1,0,0,-1,0]^T, \\ v_4 &= [1,1,1,1,-1,-1,-1,-1,1,1,1,-2,0,0,0,-1].^T \end{aligned}$$

Assume v is a $(1,-1)$-eigenvector of $\tilde{C}_4$ associated to eigenvalue 2, then it can be written as a linear combination of the above four vectors, say $v = av_1 + bv_2 + cv_3 + dv_4$. From the first two components we have $d = \pm 1$ and $-c + d = \pm 1$; therefore $c = d \pm 1 \in \{0, 2, -2\}$. But the 15th component inplies $c = \pm 1$, hence no linear combination of the four vectors is a vector that only contains entries 1 or -1. Therefore $\tilde{C}_4$ does not have a $(1,-1)$-eigenvector associated to eigenvalue 2, and therefore it is not Hadamard diagonalizable. $\square$

Now we generalize this property to $\tilde{Q}_n$.

Theorem 5.2.5. *For $n \geq 4$, the adjacency matrix $\tilde{C}_n$ of $\tilde{Q}_n$ is not Hadamard diagonalizable. In fact, $\tilde{C}_n$ has only $n-4$ linearly independent $(1,-1)$-eigenvectors associated to the eigenvalue $n-2$.*

Proof. We proceed by induction on n. From Lemma 5.2.4, we know that the number of $(1,-1)$-eigenvectors of $\tilde{C}_4$ associated to eigenvalue 2 is 0, which equals $4-4$, and the result is true for $n=4$. Assume the result is true for some integer $k \geq 4$, that is, $\tilde{C}_k$ has exactly $k-4$ linearly independent $(1,-1)$-eigenvectors associated to eigenvalue $k-2$. Let $x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ be a $(1,-1)$-eigenvector of $\tilde{C}_{k+1}$ associated to eigenvalue $(k+1)-2$, where both x_1 and x_2 are $(1,-1)$ column vectors of length 2^k. Then $\begin{bmatrix} \tilde{C}_k & I_{(k)} \\ I_{(k)} & \tilde{C}_k \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = (k-1) \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$. Therefore $\tilde{C}_k x_1 + x_2 = (k-1)x_1,$ and $x_1 + \tilde{C}_k x_2 = (k-1)x_2$, which imply

$$\left[(k-1)I_{(k)} - \tilde{C}_k\right] x_1 = x_2, \tag{5.1}$$

$$\left[(k-1)I_{(k)} - \tilde{C}_k\right] x_2 = x_1. \tag{5.2}$$

Substituting equation (5.1) into equation (5.2) gives $[(k-1)I_{(k)} - \tilde{C}_k]^2 x_1 = x_1$, so $[\tilde{C}_k^2 - 2(k-1)\tilde{C}_k + (k^2-2k)I_{(k)}]x_1 = \mathbf{0}$, i.e., x_1 is an eigenvector of $\tilde{C}_k^2 - 2(k-1)\tilde{C}_k + (k^2-2k)I_{(k)}$ associated to eigenvalue 0. Recall the fact that if the spectrum of $\tilde{C}_k$ is $\sigma(\tilde{C}_k) = \{\lambda_1, \cdots, \lambda_{2^k}\}$, then $\sigma(\tilde{C}_k^2 - 2(k-1)\tilde{C}_k + (k^2-2k)I_{(k)}) = \{\lambda_1^2 - 2(k-1)\lambda_1 + (k^2-2k), \cdots, \lambda_{2^k}^2 - 2(k-1)\lambda_{2^k} + (k^2-2k)\}$, with each eigenvector of $\tilde{C}_k$ associated to eigenvalue λ_j being an eigenvector of $\tilde{C}_k^2 - 2(k-1)\tilde{C}_k + (k^2-2k)I_{(k)}$ associated to eigenvalue $\lambda_j^2 - 2(k-1)\lambda_j + (k^2 - 2k)$. Therefore for some eigenvalue λ of $\tilde{C}_k$, $\lambda^2 - 2(k-1)\lambda + (k^2 - 2k) = 0$ holds, which implies $\lambda = k$ or $\lambda = k - 2$, and every eigenvector of $\tilde{C}_k^2 - 2(k-1)\tilde{C}_k + (k^2 - 2k)I_{(k)}$ associated to 0 is a linear combination of eigenvectors of $\tilde{C}_k$ associated to k or $k-2$. Thus x_1 can be expressed as $x_1 = a\mathbf{1}_{(k)} + by$, where y is an eigenvector of $\tilde{C}_k$ associated to $k-2$ and $\mathbf{1}_{(k)}$ is the (unique up to a scalar multiple) eigenvector of $\tilde{C}_k$ associated to eigenvalue k. Substituting $x_1 = a\mathbf{1}_{(k)} + by$ into (5.1), we have $x_2 = -a\mathbf{1}_{(k)} + by$. There are two cases. If $a \neq 0$, then $x_1 \neq x_2$ (in fact, x_1 and x_2 differ in every coordinate); since they are both $(1,-1)$-vectors, $x_1 = -x_2$. Thus $\mathbf{0} = x_1 + x_2 = a\mathbf{1}_{(k)} + by - a\mathbf{1}_{(k)} + by = 2by$, which implies that $b = 0$ (since $y \neq \mathbf{0}$) and $x_1 = a\mathbf{1}_{(k)}$. Thus $a = \pm 1$, and there is one $(1,-1)$-eigenvector $x_0 = \begin{bmatrix} \mathbf{1}_{(k)} \\ -\mathbf{1}_{(k)} \end{bmatrix}$ (or its negative) of $\tilde{C}_{k+1}$ associated to $k-1$. If $a = 0$, then $x_1 = x_2 = by$. By the inductive hypothesis, there are exactly $k-4$ such linearly independent $(1,-1)$-eigenvectors by of $\tilde{C}_k$ associated to the eigenvalue $k-2$, and so the vectors $\begin{bmatrix} by \\ by \end{bmatrix}$ form $k-4$ linearly independent eigenvectors of $\tilde{C}_{k+1}$ associated to eigenvalue $k-1$, and they are linearly independent from x_0. Altogether, we have $k-4+1 = (k+1)-4$ linearly independent $(1,-1)$-eigenvectors associated to eigenvalue $k-1$. By mathematical induction, the result is true for all $n \geq 4$.

$\square$

5.3 Partial Switching and PST

In Section 5.2, we explored the application of GM switching to the n-cube to produce the switched n-cube. In this section, we continue to use the Cartesian product construction of the n-cube ($Q_n = Q_{n-4} \square Q_4$) so that the corresponding adjacency matrix is seen to be a block matrix, with each block of size 16×16, and the diagonal blocks are all equal to the adjacency matrix C_4 of Q_4. We then perform GM switching to some (but not all) copies of (the induced subgraph) Q_4 (according to partition π of this copy of Q_4 as shown in Figure 5.1) inside the n-cube, i.e., some diagonal blocks of C_n are changed from C_4 to $\tilde{C}_4$. We call this a *partial switching*, and we analyse the PST property of these partially switched n-cubes.

5.3.1 Construction

Let $n \geq 4$. Let $A_{n,1} = C_n$ be the adjacency matrix of the n-cube, and let $A_{n,2} = \tilde{C}_n$ be the adjacency matrix of the switched n-cube, with

$$A_{4,1} = C_4 \quad = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}, \text{ and}$$

$$A_{4,2} = \tilde{C}_4 \quad = \begin{bmatrix} 0 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}.$$

The n-cube Q_n, as mentioned earlier, is the graph $Q_{n-4}\square Q_4$, with adjacency matrix $A_{n,1} = A_{n-4,1}\otimes I_{(4)} + I_{(n-4)}\otimes A_{4,1} = \operatorname{diag}(A_{4,1}, \cdots, A_{4,1}) + A_{n-4,1}\otimes I_{(4)}$. For example, $A_{5,1} = \begin{bmatrix} A_{4,1} & I_{(4)} \\ I_{(4)} & A_{4,1} \end{bmatrix}$, and $A_{6,1} = \begin{bmatrix} A_{4,1} & I_{(4)} & I_{(4)} & 0 \\ I_{(4)} & A_{4,1} & 0 & I_{(4)} \\ I_{(4)} & 0 & A_{4,1} & I_{(4)} \\ 0 & I_{(4)} & I_{(4)} & A_{4,1} \end{bmatrix}$. For the switched n-cube, we just need to replace every occurrence of $A_{4,1}$ with $A_{4,2}$. Now if we replace some of the diagonal blocks $A_{4,1}$ in $A_{n,1}$ by $A_{4,2}$, we get the adjacency matrix of a partially switched n-cube. For $n = 5$, by a simple reordering of the copies of $A_{4,1}$ and $A_{4,2}$, it is clear that $A_{5,3} = \begin{bmatrix} A_{4,1} & I_{(4)} \\ I_{(4)} & A_{4,2} \end{bmatrix}$ and $\begin{bmatrix} A_{4,2} & I_{(4)} \\ I_{(4)} & A_{4,1} \end{bmatrix}$ are isomorphic, but they are not isomorphic to the 5-cube or the switched 5-cube (by checking that $A_{5,1}$ and $A_{5,3}$ have different spectra or by the result of Example 5.3.8 in Section 5.3.3 below, which shows that there are fewer vertices in $A_{5,3}$ than in $A_{5,1}$ involved in PST). For $n = 6$, there is a unique (up to isomorphism, which can be accomplished by reordering the copies of $A_{4,1}$ and $A_{4,2}$) partially switched 6-cube with exactly one copy of the 4-cube, say $A_{6,3} = \operatorname{diag}(A_{4,1}, A_{4,2}, A_{4,2}, A_{4,2}) + A_{2,1}\otimes I_{(4)}$ and a unique (again, up to isomorphism) partially switched 6-cube with three copies of the 4-cube, say $A_{6,4} = \operatorname{diag}(A_{4,2}, A_{4,1}, A_{4,1}, A_{4,1}) + A_{2,1}\otimes I_{(4)}$; furthermore, $\Gamma(A_{6,4})$ can be obtained from $\Gamma(A_{6,3})$ by performing GM switching with respect to the partition π_2, as described in Section 5.2.1 for a general (switched, partially switched) n-cube, of the vertex set of $\Gamma(A_{6,3})$, where $\Gamma(A)$ denotes the graph with adjacency matrix A. When there are two copies of $A_{4,1}$ and two copies of $A_{4,2}$, there are two non-isomorphic partially switched 6-cubes: $A_{6,5} = \operatorname{diag}(A_{4,1}, A_{4,1}, A_{4,2}, A_{4,2}) + A_{2,1}\otimes I_{(4)}$, $A_{6,6} = \operatorname{diag}(A_{4,1}, A_{4,2}, A_{4,2}, A_{4,1}) + A_{2,1}\otimes I_{(4)}$, and these two graphs are not even cospectral. For $n \geq 7$, there are more non-isomorphic partially switched n-cubes.

The partially switched n-cubes are not cospectral to the n-cube in general, but still exhibit PST (though the number of PST vertex pairs is significantly fewer than that in the n-cube), and are not cubelike graphs, for the following reason. Consider the binary labelling of a (switched, partially switched) n-cube: every vertex has a label of the form xy, where $x \in \mathbb{Z}_2^{n-4}$ indicates the different copies of the 4-cube or switched 4-cube, and $y \in \mathbb{Z}_2^4$ represents the vertices within each copy. Note that for a fixed vertex v in the n-cube, any two neighbours of v have exactly one other common neighbour. Since for any $x \in \mathbb{Z}_2^{n-4}$, the (partial) switching does not change the graph induced by the set of vertices at distance at most 2 to $x1111$, any two neighbours of vertex $x1111$ have exactly one other common neighbour. Let x take some value such that the corresponding copy of the 4-cube is a switched one. Then the two neighbours $x0100$ and $x1011$ of the vertex $x0011$ have two other common neighbours: $x1010$ and $x1001$ (see Figure 5.3). Therefore, there is no isomorphism of a partially switched n-cube that maps vertex $x1111$ to vertex $x0011$, which shows that the graph is not vertex-transitive. Hence it is not a cubelike graph (as mentioned in Section 2.5.2, cubelike graphs are Cayley graphs, and Cayley graphs are vertex-transitive).

5.3.2 Some spectral properties of the switched n-cubes

Although partially switched n-cubes are less structured compared to the n-cube and the switched n-cube, they do share some common eigenvalues and eigenvectors. For example, they all have $n-2$ as an eigenvalue, and some common eigenvectors associated to this eigenvalue.

Proposition 5.3.1. *For $n \geq 4$, the n-cube, switched n-cube, and any partially switched n-cube have at least $n-3$ linearly independent common eigenvectors associated to the eigenvalue $n-2$.*

Proof. We prove this by induction. If $n=4$, by comparing the reduced row-echelon form (RREF) of $A_{4,1}-2I_{(4)}$ with the RREF of $A_{4,2}-2I_{(4)}$, we know that they have exactly one (up to a scalar multiple) common eigenvector associated to eigenvalue 2, which is $v=[2,1,1,1,1,0,0,0,0,0,0,-1,-1,-1,-1,-2]^T$. Hence the result is true for $n=4$. Assume that it is true for $k \geq 4$, and that $v_1^{(k)}, \ldots, v_{k-3}^{(k)}$ is a set of linearly independent common eigenvectors for the (switched, partially switched) k-cube associated to eigenvalue $k-2$. The adjacency matrix of the (switched, partially switched) $(k+1)$-cube can be written as $M = \begin{bmatrix} M_1 & I_{(k)} \\ I_{(k)} & M_2 \end{bmatrix}$, where M_1 and M_2 are the adjacency matrices of some (switched, partially switched) k-cubes according to the structure of M. By assumption, the above vectors $v_j^{(k)}$ are eigenvectors of M_1 and M_2 associated to the eigenvalue $k-2$. For $j=1,\ldots,k-3$, let $v_j^{(k+1)} = \begin{bmatrix} v_j^{(k)} \\ v_j^{(k)} \end{bmatrix}$, then direct computation shows that $v_1^{(k+1)}, \ldots, v_{k-3}^{(k+1)}$ are linearly independent eigenvectors of M associated to the eigenvalue $k-1=(k+1)-2$, and there are $k-3$ of them. Also note that $\mathbf{1}_{(k)}$ is a common eigenvector of the (switched, partially switched) k-cube associated to eigenvalue k. Hence $v_0^{(k+1)} = \begin{bmatrix} \mathbf{1}_{(k)} \\ -\mathbf{1}_{(k)} \end{bmatrix}$ is an eigenvector of M associated to the eigenvalue $k-1=(k+1)-2$. Combining the above, we get $k-3+1=(k+1)-3$ linearly independent common eigenvectors associated to eigenvalue $(k+1)-2$ of the (switched, partially switched) $(k+1)$-cube. Hence the result is true for any $k \geq 4$. $\square$

Remark 5.3.2. From the above proof it follows that the vectors $a_1 \otimes a_2 \cdots \otimes a_{n-4} \otimes \mathbf{1}_{16}$, where exactly one of $a_1, \ldots, a_{n-4}$ is $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$, and the remaining are $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$, are linearly independent (1,-1) eigenvectors (there are $n-4$ of them) associated to eigenvalue $n-2$ of the (switched, partially switched) n-cubes. By Theorem 5.2.5 we know that those are in fact all the $(1,-1)$ eigenvectors of the switched n-cube associated to the eigenvalue $n-2$. (The above theorem also tells us that a $(n-3)$-th common eigenvector of the (switched, partially switched) n-cubes is $\mathbf{1}_{(n-4)} \otimes v$, where v is a common eigenvector of the 4-cube and the switched 4-cube as given at the beginning of the proof.) Similarly, when there is exactly one $\begin{bmatrix} 1 \\ 1 \end{bmatrix}$ and $(n-5)$ many $\begin{bmatrix} 1 \\ -1 \end{bmatrix}$ in the above tensor product, we obtain eigenvectors associated to the eigenvalue $-(n-2)$ of these cubes.

Example 5.3.3. For the n-cube, the switched n-cube, or a partially switched n-cube, some of their eigenvalues and eigenvectors can be calculated from some matrices of smaller size ($3 \times 2^{n-4}$ instead of $16 \times 2^{n-4}$).

For the Hadamard matrix

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

direct computation shows that

$$\begin{aligned}
D &= H^{-1}A_{4,1}H = \operatorname{diag}(4,2,2,2,2,0,0,0,0,0,0,-2,-2,-2,-2,-4), \text{ and} \\
B &= H^{-1}A_{4,2}H = \begin{bmatrix} 4 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{2}J_4 & X & 0 & 0 \\ 0 & X^T & 0 & Y & 0 \\ 0 & 0 & Y^T & -\frac{1}{2}J_4 & 0 \\ 0 & 0 & 0 & 0 & -4 \end{bmatrix},
\end{aligned}$$

where the diagonal blocks of B are of size 1, 4, 6, 4, 1, respectively (note that these block sizes match the multiplicity of the diagonal entries of D), and

$$X = \frac{1}{2}\begin{bmatrix} -1 & -1 & 1 & -1 & 1 & 1 \\ -1 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & 1 & -1 & -1 & -1 \end{bmatrix}, Y = \frac{1}{2}\begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \\ -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ -1 & -1 & 1 & 1 \end{bmatrix}.$$

Observe that each block of B (or D) has constant row sums. Consider the partially switched 5-cube $A_{5,3} = \begin{bmatrix} A_{4,1} & I_{(4)} \\ I_{(4)} & A_{4,2} \end{bmatrix}$. Then $\begin{bmatrix} H & 0 \\ 0 & H \end{bmatrix}^{-1} A_{5,3} \begin{bmatrix} H & 0 \\ 0 & H \end{bmatrix} = \begin{bmatrix} D & I_{(4)} \\ I_{(4)} & B \end{bmatrix} =$

$A'_{5,3}$.

The vectors $a = [1, -3, 1, 1]^T$, $b = [1, -1, 1, -1, 1, -1]^T$, $c = [1,\ 1, -3, 1]^T$ satisfy $Xb = a, X^T a = 2b, Yc = 2b$, and $Y^T b = c$. Then for scalars $x_1, \ldots, x_6$, the vector $[0, x_1 a^T, x_2 b^T, x_3 c^T, 0, 0, x_4 a^T, x_5 b^T, x_6 c^T, 0]^T$ is an eigenvector of $A'_{5,3}$ associated to the eigenvalue λ if and only if $[x_1, x_2, \ldots, x_6]^T$ is an eigenvector of $T = \begin{bmatrix} T_1 & I_3 \\ I_3 & T_2 \end{bmatrix}$ associated to the eigenvalue λ, where $T_1 = \begin{bmatrix} 2 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -2 \end{bmatrix}$ and $T_2 = \begin{bmatrix} 0 & 1 & 0 \\ 2 & 0 & 2 \\ 0 & 1 & 0 \end{bmatrix}$.

Thus the eigenvalues of the 6×6 matrix $T = \begin{bmatrix} T_1 & I_3 \\ I_3 & T_2 \end{bmatrix}$ are eigenvalues of the 32×32 matrix $A_{5,3}$, and with its eigenvectors we can recover some of the corresponding eigenvectors of $A_{5,3}$ by using the vectors a, b, c, and the Hadamard matrix H.

We can also make use of other vector triples, e.g.

$$\begin{aligned} a &= [-3, 1, 1, 1]^T, b = [1, 1, -1, 1, -1, -1]^T, c = [1, 1, 1, -3]^T, \quad \text{or} \\ a &= [-1, -1, 3, -1]^T, b = [1, -1, -1, 1, 1, -1]^T, c = [-1, 3, -1, -1]^T; \end{aligned}$$

the equations above involving multiplications with X, X^T, Y, Y^T hold for each of the new vector triples a, b, c. So for any eigenvalue of $A_{5,3}$ that is also an eigenvalue of T, its multiplicity is at least 3.

In general, for a (switched, partially switched) n-cube with adjacency matrix $M = \operatorname{diag}(M_1, \cdots, M_{2^{n-4}}) + C_{n-4} \otimes I_{(4)}$, where each M_j represents $A_{4,1}$ or $A_{4,2}$, using the the above vectors a, b, and c, we can find some of its eigenvalues from a matrix of size $3 \times 2^{n-4}$, by replacing $A_{4,1}$ with T_1, $A_{4,2}$ with T_2, and $I_{(4)}$ with I_3.

5.3.3 Which vertices maintain PST?

Let $S = \{1+2^4m_4+\cdots+2^{n-1}m_{n-1}, 16+2^4m_4+\cdots+2^{n-1}m_{n-1} \,|\, m_k \in \{0,1\}$ for $k = 4,\cdots,n-1\}$. Note that S is exactly the set of singleton vertices of the partition π_1 (end of Section 5.2.1) of the vertex set $\mathbb{Z}_2^n$ of the (switched, partially switched) n-cube. We give two different approaches for the result of PST properties of vertices in S.

Theorem 5.3.4. *Let $n > 4$. Then for any given partially switched n-cube, at least 1/8 of its vertices pair up to exhibit PST at time $\pi/2$. Specifically, for any partially switched n-cube, all the vertices in the set S above pair up to exhibit PST, with PST between vertices $1+2^4m_4+2^5m_5+\cdots+2^{n-2}m_{n-2}+2^{n-1}m_{n-1}$ and $16+2^4(1-m_4)+2^5(1-m_5)+\cdots+2^{n-2}(1-m_{n-2})+2^{n-1}(1-m_{n-1})$, where $m_j \in \{0,1\}$ for $j = 4,\ldots,n-1$. Furthermore, at any time t, the fidelity of state transfer from vertex $j \in S$ to any other vertex is the same for any partially switched n-cube as it is for the n-cube.*

First we give a proof by considering the corresponding entries in the unitary matrix $e^{i(\pi/2)A}$, where A is the adjacency matrix of a given partially switched n-cube.

Proof. By direct computation, we know $e_1^TA_{4,1}^k = e_1^TA_{4,2}^k$ for $k = 1,2,3,4$. Since $A_{4,1}$ and $A_{4,2}$ have the same minimal polynomial x^5-20x^3+64x, we know $e_1^TA_{4,1}^k = e_1^TA_{4,2}^k$ for any positive integer k, i.e., for any positive integer k, $A_{4,1}^k$ and $A_{4,2}^k$ have the same first row. Similarly, they have the same 16-th row. Therefore, for any list of nonnegative integers

$j_1, j_2, \cdots, j_{2s}$, the matrix $A_{4,1}^{j_1} A_{4,2}^{j_2} A_{4,1}^{j_3} \cdots A_{4,2}^{j_{2s}}$ has the same first row as $A_{4,1}^{j_1+\cdots+j_{2s}}$, since

$$\begin{aligned} e_1^T A_{4,1}^{j_1} A_{4,2}^{j_2} A_{4,1}^{j_3} \cdots A_{4,2}^{j_{2s}} &= e_1^T A_{4,2}^{j_1} A_{4,2}^{j_2} A_{4,1}^{j_3} \cdots A_{4,2}^{j_{2s}} = e_1^T A_{4,2}^{j_1+j_2} A_{4,1}^{j_3} \cdots A_{4,2}^{j_{2s}} \\ &= e_1^T A_{4,1}^{j_1+j_2+j_3} \cdots A_{4,2}^{j_{2s}} = \cdots \\ &= e_1^T A_{4,1}^{j_1+j_2+j_3+\cdots+j_{2s}}. \end{aligned}$$

As mentioned earlier, for $n > 4$, the adjacency matrix of a partially switched n-cube is of the form $A_{n,p} = \operatorname{diag}(A_{4,*}, \cdots, A_{4,*}) + A_{n-4,1} \otimes I_{(4)}$, where $A_{n-4,1}$ is the adjacency matrix of the $(n-4)$-cube, and $*$ represents 1 or 2. For any positive integer k, each block (of size 16×16) of the matrix $A_{n,p}^k$ is of the form $\sum c(j_1, j_2, \ldots, j_{2s}) A_{4,1}^{j_1}\ A_{4,2}^{j_2} \cdots A_{4,2}^{j_{2s}}$ for some nonnegative integers $j_1, \cdots j_{2s}$ and some real number $c(j_1, j_2, \ldots, j_{2s})$, which has the same first row as $\sum c(j_1, j_2, \ldots, j_{2s}) A_{4,1}^{j_1+\cdots+j_{2s}}$, the corresponding block in $A_{n,1}^k$. Therefore $e_\ell^T A_{n,p}^k = e_\ell^T A_{n,1}^k$ for any $\ell \in \{1, 16, 2^4+1, 2^4+16, 2^5+1, 2^5+16, 2^5+2^4+1, 2^5+2^4+16 \cdots\} = S$ (these rows correspond to the first and 16-th vertices, i.e., the two singletons, in each copy of the 4-cube or the switched 4-cube). Hence for the unitary matrices $U_{n,p}(t) = e^{itA_{n,p}} = \sum_{j=0}^{\infty} \frac{(itA_{n,p})^j}{j!}$ for $A_{n,p}$ and $U_{n,1}(t) = e^{itA_{n,1}}$ for $A_{n,1}$, $e_\ell^T U_{n,p}(t) = e_\ell^T U_{n,1}(t)$ for any $\ell \in S$ and any time t. As a result, at any time t, each of the vertices in the set S has the same probability of state transfer to any other vertex as it has in the n-cube. In the n-cube, there is PST between any two vertices at distance n at time $t = \pi/2$, which correspond to vertices k and $2^n + 1 - k$ in our ordering of vertices, i.e., $|e_k^T U_{n,1}(\pi/2) e_{2^n+1-k}| = 1$. Therefore, in any partially switched n-cube, there is PST between vertices $1 + 2^4 m_4 + 2^5 m_5 + \cdots + 2^{n-2} m_{n-2} + 2^{n-1} m_{n-1}$ and

$16 + 2^4(1 - m_4) + 2^5(1 - m_5) + \cdots + 2^{n-2}(1 - m_{n-2}) + 2^{n-1}(1 - m_{n-1})$ at time $\pi/2$, where $m_j \in \{0, 1\}$ for $j = 4, \ldots, n-1$. $\square$

Now we give a different proof of the PST pair result by using the symmetrized quotient graph of a partially switched n-cube with respect to the equitable π_1 as mentioned in Remark 5.2.1.

Second proof of Theorem 5.3.4: Consider the equitable partition π_1 of $V(Q_n)$ and of the vertex set of the given partially switched n-cube. The two graphs have the same symmetrized quotient graphs with respect to π_1, and every vertex in the set S forms a singleton cell in both graphs with respect to this partition. Combining the fact that the n-cube exhibits PST between the antipodal vertices and Theorem 2.3.6, the result follows.

$\square$

Remark 5.3.5. Using the symmetrized quotient graph of Q_n with respect to the equitable partition π_1 approach, we can construct more graphs from Q_n with PST between vertices in the set S. Take the Cartesian product construction of the n-cube: $Q_n = Q_{n-4} \square Q_4$; to construct a switched n-cube, for each of the 2^{n-4} copies of Q_4, we either keep it or replace it by $\tilde{Q}_4$. Now if we replace the biregular graph induced on cells D and C_2 or the one on cells C_3 and C_2 (as shown in Figure 5.1) by any one of the three non-isomorphic biregular graphs (note that G_1 and G_3 are not isomorphic, as any two of the vertices $\{1, 2, 3, 4\}$ have exactly one common neighbour, which is not true for G_3) or their variants obtained from some reordering of the vertices (G_1 is the one for the 4-cube or the switched 4-cube on cells D and C_2) shown in Figure 5.4, the resulting graph still has π_1 as an equitable partition, and its symmetrized quotient graph with respect to π_1 is the same as the one of Q_n with respect to π_1, namely $\widehat{Q_n/\pi_1}$. Therefore there is still PST between vertices j and $2^n + 1 - j$ for any $j \in S$ at time $\pi/2$ for such a perturbed n-cube. Note that if we just consider Q_4, by only making use of G_1 in Figure 5.4, there are already 6 non-isomophic graphs (including the 4-cube and the switched 4-cube) on 16 vertices that have π as an equitable partition, and $\widehat{Q_4/\pi}$ as the symmetrized quotient graph. There are 2 of them if we only make use of G_2, and 8 of them if we only use G_3. If we consider the n-cube for $n > 4$, and replace some copies of Q_4 by any variants, then for each resulting graph, there are some other new non-isomorphic graphs related to it. For example, permuting the vertices in cell C_2 of the 4-cube or its variant but keeping the edges between copies of Q_4 or its variant fixed to the position (not the vertex), gives new graphs. Similarly, take $Q_n = Q_{n-k} \square Q_k$ for some $k > 4$, and consider the distance partition π' of Q_k with respect to vertex $x\mathbf{0}_k$ ($x \in \mathbb{Z}_2^{n-k}$ indicate the copies). Replacing copies of Q_k by any of its variants that are on the same vertex set, have π' as an equitable partition, and with $\widehat{Q_k/\pi'}$ as the symmetrized quotient graph with respect to π', produces graphs with PST between the singleton cells of equitable partition of Q_n induced by π' (there are 2^{n+1-k} singleton cells, forming a subset of S).

Using the approach of checking the entries of $e^{itA_{n,p}}$ and $e^{itA_{n,1}}$, we can get information on fidelity of state transfer between vertex $j \in S$ and any other vertices; it is the same as it is in the n-cube at any time t, which can be calculated easily through $e^{itA_{n,1}} = \begin{bmatrix} \cos t & i\sin(t) \\ i\sin(t) & \cos(t) \end{bmatrix}^{\otimes n}$. On the contrary, the symmetrized quotient graph approach only

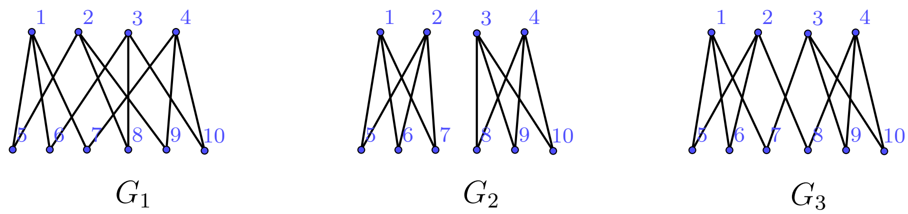


Figure 5.4: Non-isomorphic $(3, 2)$-biregular graphs on 10 vertices

tells information about fidelity between vertices in S.

Below we conjecture that the lower bound of 1/8 of the vertices in Theorem 5.3.4 is in fact exact (that is, exactly 1/8 of the vertices of partially switched n-cubes pair up to exhibit PST at time $\pi/2$). As a motivating example, we consider $A_{5,3}$, the first interesting partially switched n-cube, and verify that the bound is obtained in this case. The verification process is rather tedious, but we include the technical details for completeness. The main takeaway is that the smallest nontrivial example does indeed attain our lower bound.

Assume that G is a graph on n vertices, and its adjacency matrix has spectral decomposition $A(G) = \sum_{r=1}^{s} \lambda_r E_r$ (Theorem 2.1.2). Then for a given vertex $j \in V(G)$, its characteristic (indicator) vector is $e_j \in \mathbb{R}^n$. The *eigenvalue support* of the vertex j (or of the vector e_j) with respect to $A(G)$ is defined to be the set of eigenvalues λ_r of $A(G)$, such that $E_r e_j \neq \mathbf{0}$ [46]. Assume that G is periodic at a vertex j at some time t. Then the values in the eigenvalue support of vertex j satisfy the following ratio condition.

Theorem 5.3.6. [46, Theorem 3.1] *Let G be a graph and j be a vertex in G at which G is periodic. If θ_k, θ_ℓ, θ_r, θ_s are eigenvalues in the support of e_j and $\theta_r \neq \theta_s$, then $\frac{\theta_k - \theta_\ell}{\theta_r - \theta_s} \in \mathbb{Q}$.*

If a graph G that admits PST between vertices j and k at time t_0, then G is periodic at vertex j (and k) at time $2t_0$. Therefore if there are two integer eigenvalues in the support of j, then all the eigenvalues in the support of j are integers.

Proposition 5.3.7. *Let G be a graph on m vertices, and j be a vertex of G. Then the eigenvalue λ_r of $A(G)$ is in the eigenvalue support of e_j if and only if there is an eigenvector v_1 of $A(G)$ associated to λ_r, such that $v_1^T e_j \neq 0$.*

Proof. For any eigenvector v_1 of $A(G)$ associated to λ_r, we can extend it to $v_1, v_2, \ldots, v_k$ to get a basis of the eigenspace associated to λ_r, then by the Gram-Schmidt procedure and normalization, we can get an orthonormal basis $w_1, \ldots, w_k$ of the eigenspace, with $w_1 = \frac{1}{\|v_1\|_2} v_1$. Now $E_r e_j = (w_1 w_1^T + w_2 w_2^T + \cdots + w_k w_k^T) e_j = (w_1^T e_j) w_1 + \cdots + (w_k^T e_j) w_k$ for any vertex j, and $E_r e_j = \mathbf{0}$ if and only if $w_\ell^T e_j = 0$ for all $\ell = 1, \ldots, k$, i.e., all the eigenvectors of $A(G)$ associated to λ_r have their j-th entry equal to 0. This implies that for any eigenvalue λ_r of $A(G)$, if it has a corresponding eigenvector whose j-th entry is not 0, then λ_r is in the eigenvalue support of e_j (or of vertex j) and vice versa. $\square$

We are now in the position to consider the example of $A_{5,3}$.

Example 5.3.8. Consider $A_{5,3} = \begin{bmatrix} A_{4,1} & I_{(4)} \\ I_{(4)} & A_{4,2} \end{bmatrix}$, which has $\lambda_1 = 5$ as a simple eigenvalue, with $v_1 = \mathbf{1}_{(5)}$ being a corresponding eigenvector. By direct computation (or Remark 5.3.2), $v_2 = \begin{bmatrix} \mathbf{1}_{(4)} \\ -\mathbf{1}_{(4)} \end{bmatrix}$ is an eigenvector of $A_{5,3}$ associated to eigenvalue 3. Since all the entries of v_1 and v_2 are nonzero, from Proposition 5.3.7, $\lambda_1 = 5$ and $\lambda_2 = 3$ are both in the eigenvalue support of all the vertices.

Now let $p(\lambda) = -\lambda^6+11\lambda^4-27\lambda^2+1 = -(\lambda^3+\lambda^2-5\lambda-1)(\lambda^3-\lambda^2-5\lambda+1)$. Then $p(\lambda)$ has 6 real roots (for example, by the Intermediate Value Theorem $p(\lambda)$ has a root λ_3 in the interval $[2.7, 2.8]$). Assume the 6 roots are $\lambda_3 \geq \cdots \geq \lambda_8$; they are all eigenvalues of $A_{5,3}$, and each of them is irrational (non-integer roots of a monic integer-coefficient polynomial are irrational), with minimal polynomial either $(\lambda^3 + \lambda^2 - 5\lambda - 1)$ or $(\lambda^3 - \lambda^2 - 5\lambda + 1)$. For $k = 3, \ldots, 8$, the eigenvalue λ_k has an associated eigenvector $v(\lambda_k) = [0, a, -3a, a, a, b, -b, b, -b, b, -b, c, c, -3c, c, 0, 0, d, -3d, d, d, e, -e, e, -e, e, -e, d+4, d+4, -3(d+4), d+4, 0]^T$, where $a = 2\lambda_k(\lambda_k^4 - 10\lambda_k^2 + 17)$, $b = 8\lambda_k^2 - 8$, $c = 2\lambda_k(\lambda_k^2 - 5)^2$, $d = 2\lambda_k^4 - 12\lambda_k^2 - 6$, and $e = 8\lambda_k(\lambda_k^2 - 5)$. Note that for each $j \in T := \{1, 2, \ldots, 32\} \backslash \{1, 16, 17, 32\}$, the entry $v(\lambda_k)_j$ is not divisible by the minimal polynomial of λ_k, and therefore none of these entries are zero. Again from Proposition 5.3.7, for $k = 3, \ldots, 8$, λ_k is in the eigenvalue support of each vertex $j \in T$. Now for each $j \in T$, $\lambda_1 = 5$, $\lambda_2 = 3$, and $\lambda_3 \notin \mathbb{Q}$ are in the eigenvalue support of e_j. Since PST between vertices j and k at time t implies periodicity at vertex j (and k) at time $2t$, it follows from Theorem 5.3.6 that no vertices in the set T exhibit PST. Combining this result with Theorem 5.3.4, we obtain that the set of vertices of $A_{5,3}$ with PST is exactly $\{1, 16, 17, 32\}$.

Conjecture 5.3.9. *Let $n > 4$. For any partially switched n-cube, the set of its vertices that exhibits PST is exactly the set S we give in Theorem 5.3.4, and therefore exactly 1/8 of the vertices of a partially switched n-cube pair up to have PST.*

5.4 Other variants

5.4.1 Convex combinations

Up to now, we have been working on unweighted graphs in this chapter. In fact, some weighted n-cubes obtained from the n-cube and the switched n-cube also admit PST between certain pair of vertices. We first consider (different) convex combinations of each 4-cube or switched 4-cube block of a partially switched n-cube.

Remark 5.4.1. We can generalize partially switched n-cubes to specially weighted ones. Consider a convex combination of the 4-cube and the switched 4-cube. The resulting weighted graph G has adjacency matrix $M = pA_{4,1} + (1-p)A_{4,2}$ for $0 \leq p \leq 1$. Using the same techniques as in the proof of Theorem 5.3.4, we can see that there is perfect state transfer between vertex 1 and vertex 16. Furthermore, by induction we can see that for the weighted graph $F = Q_{n-4} \Box G$ with adjacency matrix $I_{(n-4)} \otimes M + C_{n-4} \otimes I_{(4)} = \operatorname{diag}(M, \cdots, M) + C_{n-4} \otimes I_{(4)}$, every vertex in the set S as mentioned in Theorem 5.3.4 is involved in PST. A similar statement holds for the weighted graph $\tilde{F}$ with (nonnegative) adjacency matrix $A = \operatorname{diag}(M_1, M_2, \cdots, M_{2^{n-4}}) + C_{n-4} \otimes I_{(4)}$, where $M_j = p_j A_{4,1} + (1-p_j)A_{4,2}$ with $0 \leq p_j \leq 1$ for $j = 1, \ldots, 2^{n-4}$. Note that this new family of weighted graphs contains all the other cubes as special cases: when $p_1 = \cdots = p_{2^{n-4}} = 1$, we have the n-cube, where all the vertices pair up to exhibit perfect state transfer; when $p_1 = \cdots = p_{2^{n-4}} = 0$, we have the switched n-cube, where exactly half of the vertices pair up to exhibit perfect state transfer; when $p_1, \ldots, p_{n-4} \in \{0, 1\}$ and not all of them are equal, then we have a partially switched n-cube, and Theorem 5.3.4 gives a list of vertex pairs having PST.

More generally, we can consider convex combinations of arbitrary graphs on m vertices whose adjacency matrices satisfy some specific conditions for some row.

Proposition 5.4.2. *Let $G_1, G_2, \dots, G_k$ be graphs on m vertices, whose corresponding adjacency matrices are $A(G_1), A(G_2), \dots, A(G_k)$, respectively. Suppose that for some $u \in \{1, \dots, m\}$, $e_u^T A(G_r)^j = e_u^T A(G_s)^j$ for every positive integer j and any $r, s = 1, \dots, k$. If there is PST in any one of the k graphs from vertex u to some other vertex v at time $t = t_0$, then all the other graphs have PST between vertex u and v at time t_0, as well as the weighted graph G with adjacency matrix $A = c_1 A(G_1) + \cdots + c_k A(G_k)$, where $0 \leq c_r \leq 1$ for $r = 1, \dots, k$, and $c_1 + \cdots + c_k = 1$.*

Proof. The argument is similar to the one given in Remark 5.4.1 as well as the proof of Theorem 5.3.4. In particular, we note that $A^j = (c_1 A(G_1) + \cdots + c_k A(G_k))^j$ has the same u-th row as $A(G_r)^j = (c_1 A(G_r) + \cdots + c_k A(G_r))^j$ for any nonnegative integer j and $r = 1, \dots, k$. $\square$

Corollary 5.4.3. *Any convex combination of the n-cube, the switched n-cube, some partially switched n-cube, and the weighted matrices in Remark 5.4.1, has PST between vertices $1 + 2^4 m_4 + 2^5 m_5 + \cdots + 2^{n-2} m_{n-2} + 2^{n-1} m_{n-1}$ and $16 + 2^4(1 - m_4) + 2^5(1 - m_5) + \cdots + 2^{n-2}(1 - m_{n-2}) + 2^{n-1}(1 - m_{n-1})$, at time $\pi/2$, where $m_j \in \{0, 1\}$ for $j = 4, \dots, n-1$.*

Remark 5.4.4. We already know that any convex combination of $A_{4,1}$ and $A_{4,2}$ exhibits PST between vertex 1 and 16. Here we give some spectrum properties of such convex combinations.

First, using the 4-cube and the switched 4-cube we can construct a family of positive-weighted cospectral graphs. We know from Section 2.3.2 that there is a symmetric orthogonal matrix Q such that $QA_{4,1}Q = A_{4,2}$, and $QA_{4,2}Q = A_{4,1}$. Then for any $0 \leq p \leq 1$, the weighted graphs with adjacency matrices $pA_{4,1} + (1-p)A_{4,2}$ and $pA_{4,2} + (1-p)A_{4,1}$, respectively, are cospectral to each other, and Q is the similarity matrix between the two adjacency matrices. Equivalently, we can view it in the following way: let $C = 1/2A_{4,1} + 1/2A_{4,2}$, $E = A_{4,2} - A_{4,1}$, then for any $0 \leq \alpha \leq 1/2$, the two nonnegative matrices $C + \alpha E$ and $C - \alpha E$ have the same spectrum (indeed, since $QCQ = C$ and $QEQ = -E$, we have $Q(C+\alpha E)Q = C - \alpha E$). Furthermore, the eigenvalues of $C + \alpha E$ and $C - \alpha E$ are ± 4 (with multiplicity 1), ± 2 (with multiplicity 1), 0 (with multiplicity 6), and $\sqrt{2+8\alpha^2}$ (with multiplicity 3), which can be checked by calculating the ranks of the corresponding matrices.

Similarly, for the adjacency matrix $C_n = I_{(n-4)} \otimes A_{4,1} + C_{n-4} \otimes I_{(4)}$ of Q_n, if we replace the diagonal blocks $A_{4,1}$ by different convex combinations of $A_{4,1}$ and $A_{4,2}$, then the nonnegative matrices

$$\operatorname{diag}\left(p_1 A_{4,1} + (1-p_1)A_{4,2}, p_2 A_{4,1} + (1-p_2)A_{4,2}, \cdots, p_{2^{n-4}} A_{4,1} + (1-p_{2^{n-4}})A_{4,2}\right) + C_{n-4} \otimes I_{(4)} \quad \text{and}$$

$$\operatorname{diag}\left(p_1 A_{4,2} + (1-p_1)A_{4,1}, p_2 A_{4,2} + (1-p_2)A_{4,1}, \cdots, p_{2^{n-4}} A_{4,2} + (1-p_{2^{n-4}})A_{4,1}\right) + C_{n-4} \otimes I_{(4)}$$

have the same spectrum (similar through the block diagonal matrix $\operatorname{diag}(Q, Q, \ldots, Q)$), where $0 \le p_j \le 1, j = 1, \ldots, 2^{n-4}$.

5.4.2 Switching system

As another variant, we consider switching systems where one employs a switching function to change between systems at particular times (this can be done in the absence of GM switching—it is a coincidence in naming). For example, one might use the spin network associated to the hypercube from time $t = 0$ to time $t = t_1$, then change to the spin network associated to the switched cube from time $t = t_1$ to time $t = t_2$, change to use a partially switched hypercube from time $t = t_2$ to time $t = t_3$, and so on, up to time $t_r = \pi/2$, when the n-cube, the switched n-cube, and any partially switched n-cube all have PST between pairs of vertices in the set S (as mentioned at the beginning of Section 5.3.3). We show that this new system (whose Hamiltonian changes with respect to time) has PST between vertices in the set S.

The motivation here is overcoming potential stability issues in the lab: spin networks are created in the lab with magnets and other devices and may be unstable, especially for long periods of time. Thus, one might wish to send a state along the first network until one loses confidence in the stability, then one can change to the second network and continue sending the state through this "fresh" network while rebooting the first. This would be an example of a quantum state transfer protocol requiring external modulation; such external modulation approaches typically increase the effectiveness of the state transfer, but it may be undesirable to use a protocol that relies heavily on a "hands on" approach. A switching between closely related graphs, such as between hypercubes, switched hypercubes, and partially switched hypercubes may be a useful compromise. Our approach is motivated by switched systems in control theory; see, e.g. [72].

Proposition 5.4.5. *Assume r is some positive integer. For $j = 1, \dots, r$, let G_j be any of the following: the n-cube, the switched n-cube, a partially switched n-cube, or convex combinations of the above as described in Corollary 5.4.3. If a quantum state is transferred through the network G_1 for $0 \le t \le t_1$, G_2 for $t_1 \le t \le t_2$, G_3 for $t_2 \le t \le t_3$, $\dots$, G_r for $t_{r-1} \le t \le t_r = \pi/2$, then the quantum system with time-dependent Hamiltonian $\mathcal{H}_t$ is guaranteed to have PST at time $\pi/2$ for the vertices in the set S as mentioned in Theorem 5.3.4.*

Further, if for $j = 1, \dots, r$, G_j is either the n-cube or the switched n-cube, and in addition at least one G_j is the switched n-cube, then the set of vertices exhibiting PST in this system is exactly the set of vertices exhibiting PST in the switched n-cube (one half of all the vertices).

Proof. We consider the case $r = 2$, the general case follows from induction. Fix a vertex $\ell \in S$. Then

$$\begin{aligned}
& e_\ell^T \exp\left(it_1 A(G_1)\right) \exp\left(i(t-t_1)A(G_2)\right) \\
= \;& e_\ell^T \sum_{k=0}^{\infty} \frac{(it_1)^k A(G_1)^k}{k!} \exp\left(i(t-t_1)A(G_2)\right) \\
= \;& e_\ell^T \sum_{k=0}^{\infty} \frac{(it_1)^k A(G_2)^k}{k!} \exp\left(i(t-t_1)A(G_2)\right) \text{ (by Proposition 5.4.2)} \\
= \;& e_\ell^T \exp\left(it_1 A(G_2)\right) \exp\left(i(t-t_1)A(G_2)\right) \\
= \;& e_\ell^T \exp\left(i(t_1+t-t_1)A(G_2)\right) = e_\ell^T \exp\left(itA(G_2)\right).
\end{aligned}$$

Thus the problem reduces to finding PST pairs in S for $A(G_2)$. $\square$

We now analyze the sensitivity of fidelity of state transfer, involving vertices in $S = \{1+2^4m_4+\cdots+2^{n-1}m_{n-1}, 16+2^4m_4+\cdots+2^{n-1}m_{n-1} \,|\, m_k \in \{0,1\} \text{ for } k = 4,\cdots,n-1\}$, to readout time errors in the above discussed graphs, and find that they all have the same sensitivity to readout time errors as the original hypercube when PST occurs.

5.5 Sensitivity with respect to readout time errors

Recall $S = \{1+2^4m_4+\cdots+2^{n-1}m_{n-1}, 16+2^4m_4+\cdots+2^{n-1}m_{n-1} \,|\, m_k \in \{0,1\} \text{ for } k = 4,\cdots,n-1\}$. The sensitivity of the probability (fidelity) of state transfer with respect to readout time is typically analyzed through the first derivative. An analysis of the kth derivatives (for any $k \in \mathbb{N}$) for weighted graphs with PST is given in Theorem 2.6.4. Here, we consider both the first and second derivatives.

Theorem 5.5.1. *For any PST pairs in the set S, the fidelity of state transfer between the two vertices has the same derivatives with respect to time t in the n cube, in the switched n-cube, in a partially switched n-cube and in the other n-cube variants discussed herein.*

Proof. As in Theorem 5.3.4, we have already shown that for any vertex $j \in S$, there is PST between vertex j and vertex $2^n + 1 - j$ at time $\pi/2$ for the (switched, partially switched) n-cube, and $e_j^T U_{n,p}(t) = e_j^T U_{n,1}(t) = e_j^T U_{n,2}(t)$ for any $t > 0$. Therefore the fidelity of state transfer from vertex j to any other vertex k is the same as it is in the n-cube at any time t. It follows that the three types of n-cubes have the same derivatives with respect to readout time t at any time. In particular, by Theorem 2.6.4, at time $t = \pi/2$, for the PST vertex pairs in the set S, $\frac{dp}{dt}|_{t=\frac{\pi}{2}} = 0$, and $\frac{d^2p}{dt^2}|_{t=\frac{\pi}{2}} = -2n$, where p is the fidelity of state transfer at time t between some PST vertex pair in S. Similarly, we can use the proof in Proposition 5.4.2 to prove this result for convex combinations, and use Proposition 5.4.5 to prove it for the switching system. $\square$

Chapter 6

Bounds on fidelity of state transfer with respect to readout time error or edge weight errors when PST occurs

Assume a weighted or unweighted graph G with Hamiltonian $\mathcal{H}$ exhibits PST at time t_0. As we mentioned, to achieve PST in practice, the state at the receiver needs to be read out exactly at t_0, and the spin system needs to be set up according to the parameters of G, with the interaction strength between spins j and k exactly the same as the edge weight between vertices j and k. But there may be small errors (perturbations in these parameters) in practice. We would like to make sure that even if small perturbations occur, the probability that the state read out at the receiver is the same (up to a factor) as the state sent is still very close to 1. Bounds on the fidelity of state transfer of the perturbed system, where the unperturbed system exhibits PST, are of practical use here.

In this chapter we focus on weighted graphs with PST, and take a mathematical approach to perturbations which decrease the probability of state transfer. While our approach is similar in nature to that of Kay [59] and Kirkland [66], it should be noted that other authors take different approaches. In particular, there have been a number of numerical studies investigating the robustness of fidelity with respect to perturbations (e.g. [38, 80, 89]). A recent paper of Kay [62] concerns the use of error correcting codes as a strategy for dealing with imperfections (in contrast, we do not consider encoding/decoding schemes herein).

The bounds on fidelity with respect to timing errors that we produce (for both the adjacency and Laplacian cases) look similar and in fact extend the lower bound given by Kay [59]. Moreover, we give an example where our bound is attained for the adjacency matrix case, so it cannot be further improved in that setting. Sensitivity with respect to perturbations in readout time is discussed in Section 6.1. The edge weight results are more qualitative in nature, not many bounds are known. Here we take several different approaches to get bounds on the probability of state transfer with respect to edge weight perturbations, making use of both the spectral and Frobenius norms. Sensitivity of fidelity to perturbations in edge weights is discussed in Section 6.2.

In this chapter, we consider sensitivity of the fidelity of state transfer to perturbations in readout time and in edge weight errors, when the unperturbed system exhibits perfect state transfer. All the results apart from the Laplacian dynamics results (only for weighted or unweighted graphs without loops), apply in fact to any Hamiltonian (a real symmetric matrix), weighted or unweighted graphs with or without loops. This chapter is based on work with Gordon, Kirkland, Li and Plosker [52]. The work began when Li visited the University of Manitoba in May 2015 for a one-week period. Gordon was Plosker's undergraduate student research assistant in Summer 2015.

6.1 Sensitivity to readout time

6.1.1 Fidelity of state transfer and the numerical range

Suppose G admits PST between vertices j and k at time t_0. How sensitive is $p_{j,k}(t)$ to small changes in time at time t_0? We would like $p_{j,k}(t_0+h)$ to be close to $p_{j,k}(t_0)$, which is 1, for small h. First note that we can reorder the vertices of G so that PST occurs between vertices 1 and 2. Thus we can focus on the $(1,2)$ entry of $e^{it_0\mathcal{H}}$ for simplicity and ease of notation without loss of generality, where $\mathcal{H}$ is the Hamiltonian of G under certain dynamics ($\mathcal{H}=A(G)$ if the system is governed by XY dynamics, and $\mathcal{H}=L(G)$ under Heisenberg dynamics). We also denote the fidelity of state transfer $p_{1,2}(t_0)$ as $p(t_0)$.

Since $\mathcal{H}$ is real symmetric (the adjacency matrix or Laplacian matrix of some undirected weighted graph, possibly with loops), there is a real orthogonal matrix Q that diagonalizes $\mathcal{H}$ to $\Lambda=\operatorname{diag}(\lambda_1,\ldots,\lambda_n)$: $Q^T\mathcal{H}Q=\Lambda$, where the eigenvalues λ_js satisfy $\lambda_1\leq\lambda_2\leq\ldots\leq\lambda_n$. Note that the j-th column of Q is an eigenvector of $\mathcal{H}$ associated to eigenvalue λ_j. Let $q_1^T=[q_{1,1},\ldots,q_{1,n}]$ and $q_2^T=[q_{2,1},\ldots,q_{2,n}]$ be the first two rows of

Q, that is, q_1^T (resp. q_2^T) is a row vector consisting of the first (resp. the second) entries of the eigenvectors of $\mathcal{H}$. Then $e^{it_0\mathcal{H}} = Qe^{it_0\Lambda}Q^T$. We are assuming PST between vertices 1 and 2 at time t_0, and so by Proposition 2.6.2,

$$e^{i\theta}q_1 = e^{it_0\Lambda}q_2 \tag{6.1}$$

for some $\theta \in \mathbb{R}$. In particular, for any matrix $\tilde{B} \in M_n$ and $B = \tilde{B}e^{i\theta}$,

$$|e_1^T Q\tilde{B}e^{it_0\Lambda}Q^T e_2| = |q_1^T\tilde{B}e^{it_0\Lambda}q_2| = |q_1^T\tilde{B}e^{i\theta}q_1| = |q_1^T Bq_1| = |e_1^T QBQ^T e_1|.$$

This innocuous observation will allow us to consider the $(1,1)$ entry of QBQ^T rather than the $(1,2)$ entry of $Q\tilde{B}e^{it_0\Lambda}Q^T$.

The change from the $(1,2)$ entry to the $(1,1)$ entry forges the link between the fidelity of state transfer and the notion of the *numerical range* of an $n \times n$ matrix B, defined by

$$W(B) = \{x^*Bx \,:\, x \in \mathbb{C}^n, x^*x = 1\}.$$

In particular, for any matrix B that is diagonalizable by a real orthogonal matrix Q, or more generally, by a unitary matrix, $W(B)$ is the convex hull of all the eigenvalues of B, since $W(B) = \{x^*Bx \,|\, x \in \mathbb{C}^n, x^*x = 1\} = \{x^*Q\Lambda Q^T x \,|\, x \in \mathbb{C}^n, x^*x = 1\} = \{y^*\Lambda y \,|\, y \in \mathbb{C}^n, y^*y = 1\}$, as Euclidean norm is unitary invariant, where $\Lambda = Q^T BQ$.

6.1.2 Bounds on fidelity of quantum state transfer

Theorem 6.1.1. *Let G be an undirected weighted connected graph with or without loops that admits perfect state transfer at time t_0, and $\mathcal{H}$ be its Hamiltonian under certain dynamics; that is, $p(t_0) = 1$. Suppose that there is a small perturbation and the readout* *time is $t_0 + h$ instead, with $|h| < \frac{\pi}{\lambda_n - \lambda_1}$, where, λ_1 and λ_n denote the smallest and largest eigenvalues of $\mathcal{H}$, respectively. Then the fidelity at the perturbed time $t_0 + h$ satisfies the following lower bound:*

$$p(t_0 + h) \geq \frac{1}{4}|e^{ih\lambda_1} + e^{ih\lambda_n}|^2.$$

Proof. Assume that $\mathcal{H}$ is diagonalized by a real orthogonal matrix $Q = [q_{j,k}]$ to a diagonal matrix $\Lambda = \operatorname{diag}(\lambda_1, \ldots, \lambda_n)$. Then

$$\begin{aligned} U(t_0 + h)_{1,2} &= q_1^T e^{i(t_0+h)\Lambda} q_2 = q_1^T e^{ih\Lambda} e^{it_0\Lambda} q_2 \\ &= q_1^T e^{ih\Lambda} e^{i\theta} q_1 = q_1^T B q_1 \in W(B), \end{aligned} \tag{6.2}$$

with $B = \operatorname{diag}(e^{ih\lambda_1}, \ldots, e^{ih\lambda_n})e^{i\theta}$. Note that $W(B)$ is the convex hull of $\{e^{i\theta}e^{ih\lambda_1}, \ldots, e^{i\theta}e^{ih\lambda_n}\}$. Since $|h\lambda_n - h\lambda_1| < \pi$, there exists an $s \in [0, 2\pi)$ such that $e^{is}B$ has eigenvalues $e^{i\xi_1}, \ldots, e^{i\xi_n}$ with $-\pi/2 < \xi_1 \leq \cdots \leq \xi_n < \pi/2$ and $\xi_1 = -\xi_n$. Let $e^{is}B = B_1 + iB_2$ such that $B_1 = B_1^*$ and $B_2 = B_2^*$ (i.e., the Toeplitz decomposition of $e^{is}B$ as the sum of a Hermitian matrix and a skew-Hermitian matrix [56]; in fact, $B_1 = \frac{1}{2}(e^{is}B + (e^{is}B)^*) = \operatorname{diag}(\cos\xi_1, \ldots, \cos\xi_n)$ and $B_2 = \frac{1}{2i}(e^{is}B - (e^{is}B)^*) = \operatorname{diag}(\sin\xi_1 \ldots, \sin\xi_n)$). Then the eigenvalues of B_1 satisfy $0 < \cos\xi_1 = \cos\xi_n \leq \cos\xi_j$ for all $j = 2, \ldots, n-1$. As a result, for every unit vector $x = [x_1, x_2, \ldots, x_n]^* \in \mathbb{C}^n$,

$$\begin{aligned} |x^*Bx| &= |x^*e^{is}Bx| = |x^*(B_1 + iB_2)x| \geq |x^*B_1x| \\ &= \big||x_1|^2\cos\xi_1 + \cdots + |x_n|^2\cos\xi_n\big| \geq \cos\xi_1 \\ &= |e^{i\xi_1} + e^{i\xi_n}|/2 = |e^{ih\lambda_1} + e^{ih\lambda_n}|/2, \end{aligned} \tag{6.3}$$

where the first inequality comes from the fact that $|x^*(B_1 + iB_2)x| = |\sum_j |x_j|^2\cos\xi_j +$

$i(\sum_j |x_j|^2 \sin\xi_j)| \;\geq\; |\sum_j |x_j|^2 \cos\xi_j| \;=\; |x^* B_1 x|$. Thus, every point in $W(B)$ has a distance larger than $|e^{ih\lambda_1} + e^{ih\lambda_n}|/2$ from 0. Consequently,

$$\begin{aligned} p(t_0+h) &= |U(t_0+h)_{1,2}|^2 = |q_1^T B q_1|^2 \text{ (by equation (6.2))} \\ &\geq \frac{1}{4}|e^{ih\lambda_1} + e^{ih\lambda_n}|^2 \text{ (by (6.3))} \end{aligned}$$

and the result follows. □

In fact, in the above proof, one can get a better estimate of $|q_1^* B q_1|$ using the information of $q_1 = [q_{1,1}, \ldots, q_{1,n}]^T \in \mathbb{R}^n$ and $B = \operatorname{diag}(e^{ih\lambda_1}, \ldots, e^{ih\lambda_n})e^{i\theta}$; namely, for any $s \in \mathbb{R}$,

$$\begin{aligned} |q_1^T B q_1| &= \left|\sum_{j=1}^n q_{1,j}^2 e^{i(h\lambda_j+\theta)}\right| = \left|\sum_{j=1}^n q_{1,j}^2 e^{ih(\lambda_j - s)}\right| \geq \left|\sum_{j=1}^n q_{1,j}^2 \cos(h(\lambda_j - s))\right| \\ &\geq \sum_{j=1}^n q_{1,j}^2 - \frac{h^2}{2}\sum_{j=1}^n q_{1,j}^2(\lambda_j - s)^2 \\ &= 1 - \frac{h^2}{2}\sum_{j=1}^n q_{1,j}^2(\lambda_j - s)^2, \end{aligned}$$

where the first inequality follows from the fact that $\cos(x) \geq 1 - \frac{x^2}{2}$ for any $x \in \mathbb{R}$.

In particular, if we let $s = \lambda_1$ in the above, we obtain $p(t_0+h) \geq 1 - \frac{h^2}{2}\sum_{j=1}^n q_{1,j}^2(\lambda_j - \lambda_1)^2$, a result that is parallel to the bound obtained by Kay [59], without that paper's extra hypothesis that the Hamiltonian $\mathcal{H}$ is persymmetric.

For general s, the above implies

$$\begin{aligned} p(t_0) - p(t_0 + h) &= 1 - |q_1^T B q_1|^2 \quad \text{(by (6.2))} \\ &= (1 + |q_1^T M q_1|)(1 - |q_1^T M q_1|) \\ &\le 2\left(\frac{h^2}{2}\sum_{j=1}^{n} q_{j1}^2(\lambda_j - s)^2\right) \\ &= h^2 \sum_{j=1}^{n} q_{j1}^2(\lambda_j - s)^2. \end{aligned}$$

We summarize these derivations in the following theorem.

Theorem 6.1.2. *Let G be an undirected weighted connected graph with or without loops that admits perfect state transfer at time t_0, and $\mathcal{H}$ be its Hamiltonian under certain dynamics; that is, $p(t_0) = 1$. Suppose that there is a small perturbation and the readout time is $t_0 + h$ instead, where, for the eigenvalues $\lambda_1 \le \cdots \le \lambda_n$ of $\mathcal{H}$, h satisfies $|h| < \frac{\pi}{\lambda_n - \lambda_1}$. Then, for any $s \in \mathbb{R}$, the transition probability at the perturbed time has the following lower bound:*

$$p(t_0 + h) \ge 1 - h^2 \sum_{j=1}^{n} q_{1,j}^2(\lambda_j - s)^2. \tag{6.4}$$

Theorem 6.1.2 is an improved bound compared to Theorem 6.1.1. Yet direct use of Theorem 6.1.2 requires one to find all eigenvalues $\lambda_1, \ldots, \lambda_n$ of the Hamiltonian $\mathcal{H}$, while Theorem 6.1.1 requires only that the smallest and the largest eigenvalues are known. For large spin systems, Theorem 6.1.1 would then be more practical. However, the following consequence of Theorem 6.1.2 yields a lower bound on the fidelity that involves the physical parameters of the Hamiltonian itself, and does not require any knowledge of the eigenvalues of $\mathcal{H}$.

Corollary 6.1.3. *Under the hypotheses of Theorem 6.1.2, we have*

$$p(t_0 + h) \geq 1 - h^2(e_1^T \mathcal{H}^2 e_1 - (e_1^T \mathcal{H} e_1)^2). \tag{6.5}$$

Proof. Observe that the quantity $1 - h^2 \sum_{j=1}^n q_{1,j}^2 (\lambda_j - s)^2$ in (6.4) is maximized (as a function of s) when $s \sum_{j=1}^n q_{1,j}^2 = \sum_{j=1}^n q_{1,j}^2 \lambda_j$, i.e. when $s = \sum_{j=1}^n q_{1,j}^2 \lambda_j = q_1^T \Lambda q_1 = e_1^T Q \Lambda Q^T e_1 = e_1^T \mathcal{H} e_1$. The corresponding maximum value is then $1 - h^2(\sum_{j=1}^n q_{1,j}^2 (\lambda_j - e_1^T \mathcal{H} e_1)^2) = 1 - h^2(\sum_{j=1}^n q_{1,j}^2 \lambda_j^2 - 2(e_1^T \mathcal{H} e_1) \sum_{j=1}^n q_{1,j}^2 \lambda_j + (e_1^T \mathcal{H} e_1)^2 \sum_{j=1}^n q_{1,j}^2) = 1 - h^2\big(e_1^T \mathcal{H}^2 e_1 - (e_1^T \mathcal{H} e_1)^2\big)$. Inequality (6.5) now follows readily from Theorem 6.1.2 since inequality (6.4) is true for any real number s. $\square$

Inequality (6.5) of Corollary 6.1.3 is fairly accurate in the following sense. Kirkland [66] considers the derivatives of $p(t)$ at time t_0 under the hypotheses of PST at t_0. In [66, Theorem 2.2], it is shown that all odd order derivatives of $p(t)$ at t_0 are zero, while the second derivative is equal to $-2(e_1^T \mathcal{H}^2 e_1 - (e_1^T \mathcal{H} e_1)^2))$. From [66, Theorem 2.4], it follows that the fourth derivative of p at t_0 is positive. It now follows that for all h with $|h|$ sufficiently small, there is a $c > 0$ such that $p(t_0+h) = 1-h^2(e_1^T \mathcal{H}^2 e_1 - (e_1^T \mathcal{H} e_1)^2) + ch^4 + O(h^6)$. Recall, if f is a real or complex valued function and g is a real valued function, then we write $f(x) = O(g(x))$ as $x \to a$, if and only if there exist positive numbers δ and N such that $|f(x)| \leq N g(x)$ when $0 < |x - a| < \delta$. We usually leave $x \to a$ unstated if it is clear from the context. Hence, the above discussion shows that, for small h, the lower bound of Corollary 6.1.3 is accurate to terms of order h^3.

6.1.3 The case when the bound in Theorem 6.1.1 is tight for the adjacency matrix of a weighted graph

We now consider the case where the bound in Theorem 6.1.1 is obtained when $\mathcal{H}$ is the adjacency matrix A of a connected positive-weighted graph with or without loops. For concreteness, suppose that A is of order n and that there is perfect state transfer at time t_0. Suppose A is diagonalized by a real orthogonal matrix Q to $\Lambda = \mathrm{diag}\,(\lambda_1, \ldots, \lambda_n)$ with $\lambda \leq \cdots \leq \lambda_n$. Suppose further that for some h with $|h| < \frac{\pi}{\lambda_n - \lambda_1}$, $p(t_0) - p(t_0 + h) = 1 - \frac{1}{4}|e^{ih\lambda_1} + e^{ih\lambda_n}|^2$. Denote the multiplicity of λ_1 by k, and recall that λ_n, as the Perron value of A (that is, the unique maximal eigenvalue as per the Perron-Frobenius theorem), is necessarily simple, and the Perron vector (an eigenvector associated to the Perron value), the n-th column of Q, has its entries all positive or all negative. Examining the proof of Theorem 6.1.1 (in particular, the last inequality in (6.3)), it follows that q_1 can only have nonzero entries in positions corresponding to the eigenvalues λ_j such that $\lambda_j = \lambda_1$ or $\lambda_j = \lambda_n$ (that is, $\lambda_1, \ldots, \lambda_k, \lambda_n$, by assumption). From (6.1) and the fact that $q_{1,n}$ and $q_{2,n}$ are of the same sign (therefore $q_{2,n} = q_{1,n}$), as entries of the Perron vector, it follows that $e^{i\theta}[q_{1,1}, \ldots, q_{1,k}, 0, \ldots, 0, q_{1,n}]^T = e^{it_0\Lambda}[q_{2,1}, \ldots, q_{2,k}, 0, \ldots, 0, q_{1,n}]^T$. From the facts that the corresponding entries in q_1 and q_2 are either equal or the negative of each other, $\|q_1\|_2 = \|q_2\|_2 = 1$ and that $q_1^T q_2 = 0$, it follows that $e^{i(t\lambda_j - \theta)} = -1$ and therefore $q_{2,j} = -q_{1,j}$ for $j = 1, \ldots, k$, and that $q_{1,n} = q_{2,n} \in \{\frac{1}{\sqrt{2}}, -\frac{1}{\sqrt{2}}\}$. Observe that since every column of Q has Euclidean norm 1, the n–th column of Q has nonzero entries only in its first two coordinates, but as a Perron vector for A, it cannot have any zero entries. We thus deduce that n is 2, $Q = \begin{bmatrix} \pm \begin{bmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{bmatrix}, \pm \begin{bmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{bmatrix} \end{bmatrix}$. Therefore $A = \lambda_1 \begin{bmatrix} \frac{1}{2} & -\frac{1}{2} \\ -\frac{1}{2} & \frac{1}{2} \end{bmatrix} + \lambda_2 \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} \end{bmatrix} = \frac{1}{2} \begin{bmatrix} \lambda_2 + \lambda_1 & \lambda_2 - \lambda_1 \\ \lambda_2 - \lambda_1 & \lambda_2 + \lambda_1 \end{bmatrix}$ by the spectral decomposition of A. If G doesn't have loops, A must be a positive scalar multiple of $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$. If G has loops, then the weights of loops at the two vertices need to be equal to each other.

Conversely, without loss of generality, we can assume that A is a positive scalar multiple of $\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ by Proposition 1.3.9, furthermore we assume that $A = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ by Remark 1.3.11. Then from Remark 2.1.3,

$$e^{itA} = \begin{bmatrix} \cos t & i \sin t \\ i \sin t & \cos t \end{bmatrix}.$$

At time $t = \frac{\pi}{2}$, $e^{itA} = \begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix}$ and so there is PST (since $p_{1,2}(\frac{\pi}{2}) = |i|^2 = 1$). At time $\frac{\pi}{2}+h$, the $(1,2)$ entry of $e^{i(\frac{\pi}{2}+h)A}$ is $i\sin(\frac{\pi}{2}+h) = -i\cos h = -\frac{1}{2}(e^{ih}+e^{-ih}) = -\frac{1}{2}(e^{ih\lambda_1}+e^{ih\lambda_2})$, as $\lambda_1 = -1$, and $\lambda_2 = 1$. The bound in Theorem 6.1.1 is attained.

Although Theorem 6.1.1 is true for either adjacency matrices or Laplacians, we can adapt the techniques of Theorem 6.1.1 slightly to produce an improved bound on the fidelity in the setting of the Laplacian matrix of a weighted or unweighted graph without loops, since we have more information at hand.

6.1.4 An improved bound in the case of Laplacian matrix of weighted graphs without loops

Theorem 6.1.4. *Let L be the Laplacian matrix of a connected weighted graph on $n \geq 3$ vertices. Denote the eigenvalues of L by $0 \equiv \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n$. Suppose that there is perfect state transfer at time t_0; that is, $p(t_0) = 1$. Suppose there is a small timing error, and the readout time is instead $t_0 + h$, where h satisfies $|h| < \frac{\pi}{\lambda_n}$. Then*

$$\begin{aligned} p(t_0+h) &\geq 1 - \frac{(n-1)^2(1-\cos((\lambda_n-\lambda_2)h))}{2n^2} - \frac{(n-1)(2-\cos(\lambda_2 h)-\cos(\lambda_n h))}{n^2} \\ &\quad -\frac{(\cos(\lambda_2 h)-\cos(\lambda_n h))^2}{2n^2(1-\cos((\lambda_n-\lambda_2)h)} \qquad (6.6) \\ &= \frac{\big((n-1)\sin((\lambda_n-\lambda_2)h)+\sin(\lambda_n h)-\sin(\lambda_2 h)\big)^2}{2n^2(1-\cos((\lambda_n-\lambda_2)h))}. \qquad (6.7) \end{aligned}$$

Proof. Note that the normalised all–ones vector $\frac{1}{\sqrt{n}}\mathbf{1}_n$ is a null vector for L. Assume L is diagonalized by a real orthogonal matrix Q to $\Lambda = \mathrm{diag}\,(\lambda_1, \ldots, \lambda_n)$. Then $L = Q\Lambda Q^T$ such that q_1, the first column of Q^T, has the form $[1/\sqrt{n}, x_2, \ldots, x_n]^T$, where $\sum_{j=2}^n x_j^2 = \frac{n-1}{n}$. Mimicking the proof of Theorem 6.1.1, we find that $p(t_0+h)$ is bounded below by

$$\min \left| \frac{1}{n} + z^* \mathrm{diag}\,(e^{ih\lambda_2}, \ldots, e^{ih\lambda_n}) z \right|^2,$$

where the minimum is taken over all unnormalised $z \in \mathbb{R}^{n-1}$ such that $z^*z = \frac{n-1}{n}$. From elementary geometric considerations (in short, the $e^{ih\lambda_j}$ are points on the unit circle and so the minimum will be attained by taking a convex combination of the smallest and largest values, namely $e^{ih\lambda_2}$ and $e^{ih\lambda_n}$), we find that in fact

$$\min \left| \frac{1}{n} + z^* \mathrm{diag}\,(e^{ih\lambda_2}, \ldots, e^{ih\lambda_n}) z \right|^2 =$$
$$\min_{0 \le \alpha \le \frac{n-1}{n}} \left| \frac{1}{n} + \alpha e^{ih\lambda_2} + \left(\frac{n-1}{n} - \alpha \right) e^{ih\lambda_n} \right|^2.$$

A routine calculus exercise shows that the minimum corresponds to

$$\alpha = \max \left\{ \frac{n-1}{2n} + \frac{\cos(h\lambda_n) - \cos(h\lambda_2)}{2n(1 - \cos(h(\lambda_2 - \lambda_n)))}, 0 \right\}$$

and that the minimum is given by the right hand side of (6.6).

Note that by using the formula for distance between a point and a line in the complex plane, we get bound (6.7), which is the same as the one in (6.6). $\square$

Example 6.1.5. Suppose that n is divisible by 4, and consider the unweighted graph G on n vertices formed by deleting the edge between vertices 1 and 2 from the complete graph on n vertices. Note that $L(G)$ has three eigenvalues: $\lambda_1 = 0$, with corresponding eigenprojection matrix $E_1 = \frac{1}{n} J_n$ (where J_n is the all ones matrix of size $n \times n$), $\lambda_2 = n-2$ with eigenprojection matrix $E_2 = \frac{1}{2}(e_1 - e_2)(e_1 - e_2)^T$, and $\lambda_3 = n$ with eigenprojection matrix

$$E_3 = \left[\begin{array}{c|c} \frac{n-2}{2n} J_2 & -\frac{1}{n} J_{2,n-2} \\ \hline -\frac{1}{n} J_{n-2,2} & I - \frac{1}{n} J_{n-2} \end{array} \right].$$

It is shown [69] that G admits Laplacian perfect state transfer from vertex 1 to vertex 2 at time $\frac{\pi}{2}$.

Using the eigenvalues and eigenprojection matrices above, it can be found that for any h, the fidelity at time $\frac{\pi}{2} + h$ is given by (by Remark 2.1.3)

$$p\left(\frac{\pi}{2} + h\right) = \left| \frac{1}{n} + \frac{1}{2} e^{ih(n-2)} + \frac{n-2}{2n} e^{ihn} \right|^2.$$

This last expression can be simplified to yield

$$\begin{aligned} p\left(\frac{\pi}{2}+h\right) &= 1-\frac{n-2}{2n}(1-\cos(2h))-\frac{1}{n}(1-\cos((n-2)h)) \\ &\quad -\frac{(n-2)}{n^2}(1-\cos(nh)). \end{aligned}$$

An uninteresting computation reveals that $p(\frac{\pi}{2}+h)$ exceeds the lower bound of (6.6) in the amount of

$$\frac{(\cos((n-2)h)-\cos(nh)+1-\cos(2h))^2}{2n^2(1-\cos(2h))}.$$

We note in passing that $\frac{(\cos((n-2)h)-\cos(nh)+1-\cos(2h))^2}{2n^2(1-\cos(2h))}$ is asymptotically equivalent to h^2 as $h \to 0$.

6.2 Sensitivity of fidelity to edge weights

6.2.1 A bound obtained from sensitivity of a matrix exponential to small perturbations of a Hermitian matrix

As in Section 6.1, without loss of generality we assume that there is PST between vertices 1 and 2. Here we keep the time constant at t_0, and perturb the edge weights.

Denote the (real symmetric) Hamiltonian of a system by $\mathcal{H}$. Suppose $(e^{it_0\mathcal{H}})_{1,2}$ has modulus 1; that is, the system admits PST between vertices 1 and 2 at time t_0. Consider now a perturbed system with Hamiltonian $\hat{\mathcal{H}} = \mathcal{H}+\mathcal{H}_0$, where $\mathcal{H}_0$ is a (symmetric) matrix representing small perturbations of edge weights. Mathematically, we would like to find an upper bound for $|(e^{it\mathcal{H}})_{1,2}|^2 - |(e^{it(\mathcal{H}+\mathcal{H}_0)})_{1,2}|^2$ or, when $t = t_0$,

$$1 - |(e^{it_0(\mathcal{H}+\mathcal{H}_0)})_{1,2}|^2$$

for a symmetric matrix $\mathcal{H}$ and a sufficiently small real symmetric perturbation $\mathcal{H}_0$, say, measured by the spectral norm $|||t_0\mathcal{H}_0|||_2$ or the Frobenius norm $\|t_0\mathcal{H}_0\|_F$.

Note that the entries of the matrix $\mathcal{H}_0$ represent individual edge weight errors, so our approach allows for individual edge weight perturbations rather than simply an overall (global) edge weight perturbation (where all edge weights are perturbed by e.g. 0.0001 in the same direction), or a single edge weight perturbation (where all other edge weights remain unperturbed); the latter case was the situation considered by Kirkland [66].

We begin with the following.

Theorem 6.2.1. *Suppose that perfect state transfer occurs at time t_0 for a system with Hamiltonian $\mathcal{H}$, and $\hat{\mathcal{H}} = \mathcal{H} + \mathcal{H}_0$, with a nonzero real symmetric perturbation $\mathcal{H}_0$, is the new Hamiltonian. Then*

$$\begin{aligned} 1 - |(e^{it_0(\mathcal{H}+\mathcal{H}_0)})_{1,2}|^2 &\leq 2|||t_0\mathcal{H}_0|||_2 e^{|||t_0\mathcal{H}_0|||_2} - |||t_0\mathcal{H}_0|||_2^2 e^{2|||t_0\mathcal{H}_0|||_2} \\ &\leq 2|||t_0\mathcal{H}_0|||_2 + |||t_0\mathcal{H}_0|||_2^2 - |||t_0\mathcal{H}_0|||_2^3. \end{aligned} \tag{6.8}$$

Proof. Since the Hamiltonian $\mathcal{H}$ is symmetric, from Theorem 2.1.10, we have

$$\left|\left|\left|e^{it_0(\mathcal{H}+\mathcal{H}_0)} - e^{it_0\mathcal{H}}\right|\right|\right|_2 \leq t_0|||\mathcal{H}_0|||_2 e^{t_0|||\mathcal{H}_0|||_2} \left|\left|\left|e^{it_0\mathcal{H}}\right|\right|\right|_2 = t_0|||\mathcal{H}_0|||_2 e^{t_0|||\mathcal{H}_0|||_2},$$

as $\left|\left|\left|e^{it_0\mathcal{H}}\right|\right|\right|_2 = 1$. Consequently, from the triangle inequality and Theorem 2.1.7,

$$\begin{aligned} |(e^{it_0\mathcal{H}})_{1,2}| - |(e^{it_0(\mathcal{H}+\mathcal{H}_0)})_{1,2}| &\leq |(e^{it_0(\mathcal{H}+\mathcal{H}_0)} - e^{it_0\mathcal{H}})_{1,2}| \leq \max_{j,k} |(e^{it_0(\mathcal{H}+\mathcal{H}_0)} - e^{it_0\mathcal{H}})_{j,k}| \\ &\leq \left|\left|\left|e^{it_0(\mathcal{H}+\mathcal{H}_0)} - e^{it_0\mathcal{H}}\right|\right|\right|_2 \leq t_0 |||\mathcal{H}_0|||_2 e^{t_0|||\mathcal{H}_0|||_2}. \end{aligned}$$

Therefore

$$1 - |||t_0\mathcal{H}_0|||_2 e^{|||t_0\mathcal{H}_0|||_2} \leq |(e^{it_0(\mathcal{H}+\mathcal{H}_0)})_{1,2}|.$$

For small enough $\mathcal{H}_0$ such that $|||t_0\mathcal{H}_0|||_2 e^{|||t_0\mathcal{H}_0|||_2} \leq 1$, squaring both sides and rearranging terms,

$$\begin{aligned} & 1 - |(e^{it_0(\mathcal{H}+\mathcal{H}_0)})_{1,2}|^2 \leq 2|||t_0\mathcal{H}_0|||_2 e^{|||t_0\mathcal{H}_0|||_2} - |||t_0\mathcal{H}_0|||_2^2 e^{2|||t_0\mathcal{H}_0|||_2} \\ = \; & 2|||t_0\mathcal{H}_0|||_2 (1 + \frac{|||t_0\mathcal{H}_0|||_2}{1!} + \frac{|||t_0\mathcal{H}_0|||_2^2}{2!} + \cdots) \\ & - |||t_0\mathcal{H}_0|||_2^2 (1 + \frac{2|||t_0\mathcal{H}_0|||_2}{1!} + \frac{(2|||t_0\mathcal{H}_0|||_2)^2}{2!} + \cdots) \\ \leq \; & 2|||t_0\mathcal{H}_0|||_2 + |||t_0\mathcal{H}_0|||_2^2 - |||t_0\mathcal{H}_0|||_2^3, \end{aligned}$$

so that (6.8) holds. □

We note that the estimate $\left|\left|\left|e^{it_0(\mathcal{H}+\mathcal{H}_0)} - e^{it_0\mathcal{H}}\right|\right|\right|_2 \leq |||t_0\mathcal{H}_0|||_2 e^{|||t_0\mathcal{H}_0|||_2}$ of Theorem 6.2.1 can be reasonably accurate. For example, suppose $\mathcal{H} = A$ is the adjacency matrix of a connected weighted graph with perfect state transfer at time t_0. Let v denote the positive Perron vector of A with norm one, and suppose that $\mathcal{H}_0 = A_0 = \epsilon vv^T$ for some small $\epsilon > 0$. Then $\left|\left|\left|e^{t_0(A+A_0)} - e^{it_0A}\right|\right|\right|_2 = |e^{it_0\epsilon} - 1|$ (using the facts that spectral norm is unitarily invariant and that if $\sigma(A) = \{\lambda_1, \ldots, \lambda_n\}$ with λ_n being its Perron-value, then $\sigma(A + A_0) = \{\lambda_1, \ldots, \lambda_n + \epsilon\}$, and the two matrices have the same corresponding eigenvectors), while $|||t_0A_0|||_2 e^{|||t_0A_0|||_2} = t_0\epsilon e^{t_0\epsilon}$, so that

$$\frac{\left|\left|\left|e^{it_0(A+A_0)} - e^{it_0A}\right|\right|\right|_2}{|||t_0A_0|||_2 e^{|||t_0A_0|||_2}} \to 1$$

as $\epsilon \to 0^+$.

6.2.2 An improved bound for special Hamiltonian $\mathcal{H}$ and small perturbations

If we have additional information about the Hamiltonian $\mathcal{H}$, we may be able to produce some better bounds as shown in Theorem 6.2.3 below. Before presenting the theorem, we require a preliminary proposition which is intuitively clear. Its proof consists of elementary linear algebra manipulation techniques; we give the proof for completeness.

Proposition 6.2.2. *Suppose that the system with Hamiltonian $\mathcal{H}$ admits perfect state transfer between vertices 1 and 2 at time t_0; that is, $|(e^{it_0\mathcal{H}})_{1,2}| = 1$. Then for some $\theta \in \mathbb{R}$ and a real orthogonal matrix $\tilde{Q}$, $t_0\mathcal{H} = \tilde{Q}\tilde{D}\tilde{Q}^T + \theta I$, where*

$$\tilde{D} = \pi\mathrm{diag}\left(r_1, \ldots, r_\ell, r_{\ell+1}, \ldots, r_m, r_{m+1}, \ldots, r_n\right)$$

such that $r_1 \geq \cdots \geq r_\ell$ are positive even integers, and $r_{\ell+1} \geq \cdots \geq r_m$ are positive odd integers. Further, the first two rows of $\tilde{Q}$ can be taken to have the form $[x_1, \ldots, x_m, 0, \ldots, 0]$ and $[x_1, \ldots, x_\ell, -x_{\ell+1}, \ldots, -x_m, 0, \ldots, 0]$ satisfying $x_1, \ldots, x_m \geq 0$.

Proof. As in Section 6.1, assume $\mathcal{H}$ is diagonalized by a real orthogonal matrix Q to a real diagonal Λ, that is, $\mathcal{H} = Q\Lambda Q^T$. Suppose that the first two rows of Q are q_1^T and q_2^T.

Then, by Proposition 2.6.2, PST between vertex 1 and vertex 2 implies that $e^{it_0\Lambda}q_2 = e^{i\theta}q_1$ or, equivalently, $e^{-i\theta}e^{it_0\Lambda}q_2 = q_1$ (or $q_2^Te^{-i\theta}e^{it_0\Lambda} = q_1^T$) for some $\theta \in \mathbb{R}$. Therefore the corresponding entries of q_1 and q_2 have the same absolute value, in particular, the j-th entry of q_1 is zero if and only if the j-th entry of q_2 is zero. For a suitable permutation matrix P_1 we can replace (Λ, Q) by $(P_1^T\Lambda P_1, QP_1)$ so that the zero entries of $q_1^TP_1$ all occur in the last $n-m$ entries, for some $0 < m \le n$. In this way, we may assume that $P_1^T(t_0\Lambda - \theta I)P_1$ is a diagonal matrix with diagonal entries of the form $s_1\pi, \ldots, s_m\pi, *, \ldots, *$ for some integers $s_1, \ldots, s_m$. The asterisks in the $(m+1, m+1)$ up to (n, n) entries of the diagonal matrix $P_1^T(t_0\Lambda - \theta I)P_1$ represent unknown constants, corresponding to the zero entries (if any) of $q_1^TP_1$. We can replace θ by $\theta - 2s\pi$ for a sufficiently large integer s so that we may assume that $s_1, \ldots, s_m$ are positive integers.

Next, for a suitable permutation matrix P_2 we can replace the pair $(P_1^T\Lambda P_1, QP_1)$ by $(P_2^TP_1^T\Lambda P_1P_2, QP_1P_2)$, so that $P_2^TP_1^T(t_0\Lambda - \theta I)P_1P_2 = \pi\mathrm{diag}\,(r_1, \ldots, r_n)$ with $r_1 \ge \cdots \ge r_\ell$ even, $r_{\ell+1} \ge \cdots \ge r_m$ odd, and $r_{m+1}, \ldots, r_n$ unknown constants; note that we still have $\mathcal{H} = (QP_1P_2)(P_2^TP_1^T\Lambda P_1P_2)(QP_1P_2)^T$. Further, we may replace the pair $(P_2^TP_1^T\Lambda P_1P_2, QP_1P_2)$ by $(SP_2^TP_1^T\Lambda P_1P_2S, QP_1P_2S)$ for some diagonal orthogonal matrix S, whose diagonal entries are 1 or -1, such that the first row of QP_1P_2S, namely $e_1^TQP_1P_2S = (x_1, \ldots, x_m, 0, \ldots, 0)$, satisfies $x_1, \ldots, x_m > 0$. Now rewriting $q_2^Te^{-i\theta}e^{it_0\Lambda} = e_2^TQe^{-i\theta}e^{it_0\Lambda}$ with the new real orthogonal matrix QP_1P_2S and the new diagonal matrix $SP_2^TP_1^T\Lambda P_1P_2S$ gives

$$e_2^T(QP_1P_2S)e^{-i\theta}e^{it_0SP_2^TP_1^T\Lambda P_1P_2S} = q_2^Te^{-i\theta}e^{it_0\Lambda}P_1P_2S = q_1^TP_1P_2S = e_1^T(QP_1P_2S),$$

which combined with the fact that $P_2^T P_1^T(t_0\Lambda - \theta I)P_1P_2 = \pi\mathrm{diag}\,(r_1, \ldots, r_n)$ with $r_1, \ldots, r_\ell$ even, $r_{\ell+1}, \ldots, r_m$ odd, and $r_{m+1}, \ldots, r_n$ unknown, imply that

$$e_2^T(QP_1P_2S) = [x_1, \ldots, x_\ell, -x_{\ell+1}, \ldots, -x_m, 0, \ldots, 0].$$

Relabelling $\tilde{D} = SP_2^T P_1^T(t_0\Lambda - \theta I)P_1P_2S$ and $\tilde{Q} = QP_1P_2S$ for simplicity, the result now follows. □

Theorem 6.2.3. *Suppose perfect state transfer occurs at time t_0 in a system with $n \times n$ Hamiltonian $\mathcal{H}$, and $\hat{\mathcal{H}} = \mathcal{H} + \mathcal{H}_0$, with a small nonzero real (symmetric) perturbation $\mathcal{H}_0$, is the new Hamiltonian. Furthermore, assume that the value m (for $\mathcal{H}$) in Proposition* 6.2.2 *equals n. Then*

$$1 - |(e^{it_0\hat{\mathcal{H}}})_{1,2}|^2 \leq \frac{2\|t_0\mathcal{H}_0\|_F^2}{(\pi - |||t_0\mathcal{H}_0|||_2)^2} + |||t_0\mathcal{H}_0|||_2^2 + O(|||t_0\mathcal{H}_0|||_2^3).$$

Proof. Assume $t_0\mathcal{H} = QDQ^T + \theta I$, with $D = \tilde{D} = \pi\mathrm{diag}\,(r_1, \ldots, r_\ell, r_{\ell+1}, \ldots, r_m)$, $Q = \tilde{Q}$ a real orthogonal matrix as in Proposition 6.2.2, and $m = n$. Here we drop the tilde for notational simplicity. Relabel $d_j = \pi r_j$ for $j = 1, \ldots, n$, so that $D = \mathrm{diag}\,(d_1, \ldots, d_n)$ is such that the first ℓ entries are even multiples of π and the last $n - \ell$ entries are odd multiples of π. Then $e^{iD} = I_\ell \oplus -I_{n-\ell}$, denote this matrix by $\mathcal{J}$. Note that $\mathcal{J}^{-1} = \mathcal{J}$.

Suppose that $t_0(\mathcal{H} + \mathcal{H}_0) = \hat{Q}\hat{D}\hat{Q}^T + \theta I$ for some real orthogonal matrix $\hat{Q}$ and the same θ as in $t_0\mathcal{H} = QDQ^T + \theta I$. Assume $\hat{D} = \mathrm{diag}\,(\hat{d}_1, \ldots, \hat{d}_n)$. By a suitable choice of $\hat{Q}$, we may assume that there is a permutation matrix P such that both $P^T DP$ and $P^T\hat{D}P$

have diagonal entries arranged in descending order. Then by Theorem 2.1.12,

$$\begin{aligned} \left|\left|\left| D-\hat{D} \right|\right|\right|_2 &= \left|\left|\left| P^T D P - P^T \hat{D} P \right|\right|\right|_2 \\ &\leq |||t_0\mathcal{H} - t_0(\mathcal{H}+\mathcal{H}_0)|||_2 = |||t_0\mathcal{H}_0|||_2, \end{aligned} \tag{6.9}$$

and hence

$$\left|\left|\left| e^{iD} - e^{i\hat{D}} \right|\right|\right|_2 \leq \left|\left|\left| D-\hat{D} \right|\right|\right|_2 \leq |||t_0\mathcal{H}_0|||_2, \tag{6.10}$$

where the first inequality comes from the fact that the singular values of a normal matrix are the moduli of its eigenvalues, and the fact that $|e^{ia}-e^{ib}| \leq |a-b|$ for any real numbers a and b (distance between two points on a unit circle is less than or equal to the length of the curve on the unit circle between them).

Let V be an orthogonal matrix close to I such that $\|V-I\|_F < 1$. Then by Theorem 2.1.9, we may write $\log(V)$ as a power series $\log(V) = -\sum_{j=1}^{\infty}\frac{1}{j}(I-V)^j$. Setting $K=\log(V)$, we have $e^K = V$. It follows that $I = VV^T = e^K e^{K^T} = e^{K+K^T}$, where the last equality comes from the fact that K commutes with K^T. We deduce that $K^T = -K$, i.e. K is skew–symmetric. We will use this idea in what follows.

Recall that Q (resp. $\hat{Q}$) is a real orthogonal matrix that diagonalizes $t_0\mathcal{H}$ (resp. $t_0(\mathcal{H}+\mathcal{H}_0)$) to $D+\theta I$ (resp. $\hat{D}+\theta I$) as in Proposition 6.2.2 and in Theorem 6.2.3. If $\mathcal{H}_0$ is small, we may assume that the differences between the corresponding eigenvalues and eigenspaces of $t_0(\mathcal{H}+\mathcal{H}_0)$ and $t_0\mathcal{H}$ are small so that $\hat{D}$ is close to D, and $\hat{Q}^TQ$ is close to I, by Theorem 2.1.13 and Theorem 2.1.14. As a result, we can write $\hat{D}-D = wD_1$ and $e^{wK} = \hat{Q}^TQ$ for a small positive number w, a diagonal matrix D_1 and a matrix K such that $\max\{|||D_1|||_2, |||K|||_2\} = 1$ (the norm condition is required so that the terms like $w^3q_1^TK^3q_1$, $w^3q_1^TD_1^3q_1$ can be lumped into the $O(w^3)$ term below). Now we denote the real orthogonal matrix $\hat{Q}$ that diagonalizes $t_0(\mathcal{H}+\mathcal{H}_0)$ by Q_w accordingly, using the subscript w here to emphasize the dependence on some small positive number w, therefore $Q_w^T = e^{wK}Q^T$. Note that it is possible that $D_1 = 0$ or $K = 0$ but not both as $\mathcal{H}_0 \neq 0$. We emphasize that $K = \frac{1}{w}\log(\hat{Q}^TQ)$ is skew–symmetric, from the above remark about the matrix V.

Now $t_0\hat{\mathcal{H}} = \hat{Q}(\hat{D}+\theta I)\hat{Q}^T$ and $Q_w = \hat{Q}$ imply that $t_0\hat{\mathcal{H}} - \theta I = Q_w\hat{D}Q_w^T$. Using the power series expansion of $e^{it_0\hat{\mathcal{H}}}$ and the facts that $K = -K^T$, $\hat{D} = D + wD_1$ and that $Q_w^T = e^{wK}Q^T$, we get

$$
\begin{aligned}
&e^{-i\theta}e_1^T(e^{it_0\hat{\mathcal{H}}})e_2 = e_1^T(Q_we^{i\hat{D}}Q_w^T)e_2\\
&= e_1^T\big[Q(I+wK+\frac{1}{2}w^2K^2)^Te^{iD}(I+iwD_1-w^2\frac{1}{2}D_1^2)(I+wK+\frac{1}{2}w^2K^2)\big]Q^Te_2+O(w^3)\\
&= (Qe^{iD}Q^T)_{1,2} + we_1^TQ[K^Te^{iD}+e^{iD}iD_1+e^{iD}K]Q^Te_2+\frac{1}{2}w^2e_1^TQ[(K^T)^2e^{iD}\\
&\quad - e^{iD}D_1^2+e^{iD}K^2]Q^Te_2+w^2e_1^TQ[K^Te^{iD}iD_1+K^Te^{iD}K+e^{iD}iD_1K]Q^Te_2+O(w^3).
\end{aligned}
$$

Recall that $\mathcal{J} = e^{iD} = I_\ell \oplus -I_{n-\ell}$. By the facts that $\mathcal{J}q_2 = q_1$ (therefore $q_2^T = q_1^T\mathcal{J}$ and $q_2 = \mathcal{J}q_1$), $\mathcal{J}^2 = I$, and $q^TKq = 0$ for any vector $q \in \mathbb{R}^n$ (since $q^TKq = (q^TKq)^T = q^TK^Tq = -q^TKq$), we have

$$
\begin{aligned}
&e^{-i\theta}e_1^T(e^{it_0\hat{\mathcal{H}}})e_2 = e_1^TQ_we^{i\hat{D}}Q_w^Te_2 = 1 + w(q_1^TK^Tq_1+q_2^TKq_2)+iwq_1^TD_1q_1+\frac{1}{2}w^2q_1^T((K^T)^2\\
&\quad - D_1^2+\mathcal{J}K^2\mathcal{J}+2K^T\mathcal{J}K\mathcal{J})q_1+iw^2q_1^T(K^TD_1+\mathcal{J}D_1K\mathcal{J})q_1+O(w^3)\\
&= 1+\frac{1}{2}w^2q_1^T((K^T)^2-D_1^2+\mathcal{J}K^2\mathcal{J}+2K^T\mathcal{J}K\mathcal{J})q_1+iwq_1^TD_1q_1\\
&\quad + iw^2q_1^T(K^TD_1+D_1\mathcal{J}K\mathcal{J})q_1+O(w^3).
\end{aligned}
$$

Let $x(w) = \mathrm{Re}(e_1^T Q_w e^{i\hat{D}} Q_w^T e_2)$, and $y(w) = \mathrm{Im}(e_1^T Q_w e^{i\hat{D}} Q_w^T e_2)$. Then

$$\begin{aligned}
&|e_1^T e^{it_0(\mathcal{H}+\mathcal{H}_0)} e_2|^2 - |e_1^T e^{it_0\mathcal{H}} e_2|^2 = |e_1^T e^{it_0(\mathcal{H}+\mathcal{H}_0)} e_2|^2 - 1 \\
&= x(w)^2 + y(w)^2 - 1 \\
&= w^2[q_1^T(K^2 + \mathcal{J}K^2\mathcal{J} - 2K\mathcal{J}K\mathcal{J} - D_1^2)q_1 + (q_1^T D_1 q_1)^2] + O(w^3) \\
&= -w^2\big(\|(K\mathcal{J} - \mathcal{J}K)q_1\|_2^2 + \|D_1 q_1\|_2^2 - (q_1^T D_1 q_1)^2\big) + O(w^3).
\end{aligned} \tag{6.11}$$

For the last equality in the above expression, we use the fact that, although $\mathcal{J}K\mathcal{J}K \neq K\mathcal{J}K\mathcal{J}$, it is true that $q_1^T\mathcal{J}K\mathcal{J}Kq_1 = (q_1^T\mathcal{J}K\mathcal{J}Kq_1)^T = q_1^T K^T\mathcal{J}^T K^T\mathcal{J}^T q_1 = q_1^T K\mathcal{J}K\mathcal{J}q_1$, which is all that is required here.

Now we find a upper bound for $w^2\|(K\mathcal{J} - \mathcal{J}K)q_1\|_2^2$ and for $\|D_1q_1\|_2^2 - (q_1^T D_1 q_1)^2$ from (6.11), separately. We start with the former one. Partition wK in accordance with $\mathcal{J} = I_\ell \oplus -I_{n-\ell}$ as $wK = \begin{bmatrix} K_{11} & K_{12} \\ -K_{12}^T & K_{22} \end{bmatrix}$, where K_{11} is $\ell \times \ell$. Then $wKJ - wJK = \begin{bmatrix} O & -2K_{12} \\ -2K_{12}^T & O \end{bmatrix}$ and hence

$$\|(wK\mathcal{J} - w\mathcal{J}K)q_1\|_2^2 \leq |||wKJ - wJK|||_2^2 = 4|||K_{12}|||_2^2, \tag{6.12}$$

by the inequality between Euclidean norm of a vector Ax and the spectral norm of matrix A in Theorem 2.1.7.

Now,

$$Q_w^T Q = e^{wK} = I + wK + \frac{(wK)^2}{2!} + \frac{(wK)^3}{3!} + \cdots .$$

So, $wK = (Q_w^T Q - Q^T Q_w)/2 + F$, where $|||F|||_2 = O(w^3)$. Partition F in accordance with $\mathcal{J}$ (or wK) as $F = \begin{bmatrix} F_1 & F_2 \\ F_3 & F_4 \end{bmatrix}$, then $|||F_j|||_2 = O(w^3)$ for $j = 1, \ldots, 4$.

Assume $Q_w^T Q \equiv V = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix}$ with V_{11} of size $\ell \times \ell$. Then $wK = (V - V^T)/2 + F$, $K_{12} = (V_{12} - V_{21}^T)/2 + F_2$ (with $|||F||| = O(w^3)$, $|||F|||_2 = O(w^3)$). Note that V_{12} and V_{21} have the same spectral norm and the same Frobenius norm. There are a number of ways of seeing this; perhaps the simplest is to note that since $Q_w^T Q$ is orthogonal, it follows that $V_{11}V_{11}^T + V_{12}V_{12}^T = I$ and $V_{11}^T V_{11} + V_{21}^T V_{21} = I$; that is, $V_{11}V_{11}^T = I - V_{12}V_{12}^T$ and $V_{11}^T V_{11} = I - V_{21}^T V_{21}$. Now use the facts that for any A, B^T of size $m \times n$, the two matrices AB and BA have the same set of nonzero eigenvalues and that $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$, we know that $V_{12}V_{12}^T$ and $V_{21}^T V_{21}$ have the same set of nonzero eigenvalues and that $\mathrm{Tr}(V_{12}V_{12}^T) = \mathrm{Tr}(V_{21}^T V_{21})$, that is,

$$|||V_{12}|||_2 = |||V_{21}|||_2, \|V_{12}\|_F = \|V_{21}\|. \tag{6.13}$$

Note that

$$\begin{aligned} \|t_0 \mathcal{H}_0\|_F^2 &= \|t_0(\mathcal{H} + \mathcal{H}_0) - t_0 \mathcal{H}\|_F^2 = \|Q_w(\hat{D} + \theta I)Q_w^T - Q(D + \theta I)Q^T\|_F^2 \\ &= \|Q_w \hat{D} Q_w^T - QDQ^T\|_F^2 = \|\hat{D}V - VD\|_F^2 \\ &= \sum_{j,k} (d_k - \hat{d}_j)^2 v_{j,k}^2, \end{aligned} \tag{6.14}$$

where we obtain the fourth equality by premultiplying by Q_w^T, postmultiplying by Q, and using the fact that the Frobenius norm is unitarily invariant.

Now consider indices j and k such that $1 \le j \le \ell < k \le n$ or $1 \le k \le \ell < j \le n$, The reverse triangle inequality gives us

$$\begin{aligned} |d_k - \hat{d}_j| &= |d_k - d_j + d_j - \hat{d}_j| \\ &\geq |d_k - d_j| - |d_j - \hat{d}_j| \\ &\geq \pi - \left|\left|\left| D - \hat{D} \right|\right|\right|_2 \\ &\geq \pi - |||t_0 \mathcal{H}_0|||_2 \quad \text{(by (6.9))}. \end{aligned}$$

Now for small enough $\mathcal{H}_0$ such that $|||t_0\mathcal{H}_0|||_2 < \pi$, continue with (6.14), we have

$$\begin{aligned} \|t_0\mathcal{H}_0\|_F^2 &= \sum_{j,k} (d_k - \hat{d}_j)^2 v_{j,k}^2 \\ &\geq \sum_{1\leq j\leq \ell<k\leq n} (d_k - \hat{d}_j)^2 v_{j,k}^2 + \sum_{1\leq k\leq \ell<j\leq n} (d_k - \hat{d}_j)^2 v_{j,k}^2 \\ &\geq (\pi - |||t_0\mathcal{H}_0|||_2)^2 (\|V_{12}\|_F^2 + \|V_{21}\|_F^2) = 2(\pi - |||t_0\mathcal{H}_0|||_2)^2 \|V_{12}\|_F^2 \text{ (by (6.13))}\,. \end{aligned}$$

It follows that

$$\|V_{12}\|_F^2 \leq \frac{\|t_0\mathcal{H}_0\|_F^2}{2(\pi - |||t_0\mathcal{H}_0|||_2)^2}.$$

Combining the facts that $K_{12} = (V_{12} - V_{21}^T)/2 + F_2$ (where $|||F|||_2 = O(w^3)$), equation (6.13), and the triangle inequality for matrix norm, we have

$$\begin{aligned} |||K_{12}|||_2 &\leq (|||V_{12}|||_2 + |||V_{21}|||_2 + O(w^3))/2 = |||V_{12}|||_2 + O(w^3) \leq \|V_{12}\|_F + O(w^3) \\ &\leq \frac{\|t_0\mathcal{H}_0\|_F}{\sqrt{2}(\pi - |||t_0\mathcal{H}_0|||_2)} + O(w^3), \end{aligned} \tag{6.15}$$

where the second inequality comes from Theorem 2.1.7. As a result, from (6.12) and (6.15) we have

$$w^2 \|(KJ - JK)q_1\|_2^2 \leq 4|||K_{12}|||_2^2 \leq \frac{2\|t_0\mathcal{H}_0\|_F^2}{(\pi - |||t_0\mathcal{H}_0|||_2)^2}. \tag{6.16}$$

Now we find an upper bound for $w^2\left(\|D_1q_1\|_2^2 - (q_1^TD_1q_1)^2\right)$ from (6.11). A result of Mirsky [76] states that for any Hermitian matrix M, the eigenvalue spread for M (the distance between the largest eigenvalue and smallest eigenvalue of M) is equal to $2\max|u^*Mv|$, where the maximum is taken over all pairs of orthonormal vectors u and v in $\mathbb{C}^n$. Consequently, for any symmetric matrix S, if $\{u,v\}$ is an orthonormal set, then

$$2|u^*Sv| \le \lambda_n(S) - \lambda_1(S),$$

where we recall that λ_1 is the minimum eigenvalue and λ_n is the maximum eigenvalue. In particular, if we set $S = wD_1$, $v = q_1$, and $Sq_1 = \mu_1q_1 + \mu_2q$ for some vector q and real numbers μ_1, μ_2, such that $\{q_1, q\}$ is an orthonormal set. Let $u = q$, then

$$\begin{aligned}
& \|wD_1q_1\|_2^2 - (q_1^TwD_1q_1)^2 \\
= \quad & (\mu_1q_1 + \mu_2q)^*(\mu_1q_1 + \mu_2q) - (q_1^T(\mu_1q_1 + \mu_2q))^2 \\
= \quad & \mu_2^2 = |q^T(wD_1)q_1|^2 \le ((\lambda_n(wD_1) - \lambda_1(wD_1))/2)^2.
\end{aligned}$$

Since D_1 is diagonal, its spectral norm is equal to its spectral radius, and combined with (6.9) we have

$$\begin{aligned}
&((\lambda_n(wD_1) - \lambda_1(wD_1))/2)^2 \le \max\left\{|\lambda_n(wD_1)|^2, |\lambda_1(wD_1)|^2\right\} \\
&= \|\|wD_1\|\|_2^2 = \left|\left|\left|\hat{D} - D\right|\right|\right|_2^2 \le \|\|t_0\mathcal{H}_0\|\|_2^2.
\end{aligned} \tag{6.17}$$

Combining (6.11), (6.16), and (6.17), the theorem follows. $\square$

Consider the bounds for $1 - \left|(e^{it_0(\mathcal{H}+\mathcal{H}_0)})_{1,2}\right|^2$ in Theorems 6.2.1 and in Theorem 6.2.3 when the perturbing matrix $\mathcal{H}_0$ is small so that $\|\|t_0\mathcal{H}_0\|\|_2 < 1$. The upper bound in the former result is $2|||t_0\mathcal{H}_0|||_2 + |||t_0\mathcal{H}_0|||_2^2 - |||t_0\mathcal{H}_0|||_2^3$, while the upper bound in the latter result is $\frac{2\|\mathcal{H}_0\|_F^2}{(\pi - |||\mathcal{H}_0|||_2)^2} + |||t_0\mathcal{H}_0|||_2^2 + O(|||t_0\mathcal{H}_0|||_2^3)$. Thus we find that, neglecting terms of order $|||t_0\mathcal{H}_0|||_2^3$, the bound of Theorem 6.2.3 is sharper than that of Theorem 6.2.1 provided that

$$\frac{\|t_0\mathcal{H}_0\|_F^2}{(\pi - |||t_0\mathcal{H}_0|||_2)^2} < |||t_0\mathcal{H}_0|||_2. \tag{6.18}$$

Suppose for concreteness that $\mathcal{H}_0$ has rank r. Recalling that $\|t_0\mathcal{H}_0\|_F^2 \leq r|||t_0\mathcal{H}_0|||_2^2$ from Theorem 2.1.7, we find that in order for (6.18) to hold, it is sufficient that $r|||t_0\mathcal{H}_0|||_2 < (\pi - |||t_0\mathcal{H}_0|||_2)^2$, or equivalently, that $|||t_0\mathcal{H}_0|||_2 < \frac{2\pi + r - \sqrt{4\pi r + r^2}}{2}$. It now follows that for all sufficiently small $\mathcal{H}_0$, the bound of Theorem 6.2.3 is an improvement upon that of Theorem 6.2.1. Thus, in the case that the more restrictive hypothesis of Theorem 6.2.3 holds, we get a better estimate from Theorem 6.2.3 than from Theorem 6.2.1.

Example 6.2.4. We give a small numerical example illustrating Theorem 6.2.3. Consider the 10×10 symmetric tridiagonal matrix M with $m_{j,j+1} = m_{j+1,j} = \sqrt{j(10-j)}, j = 1, \ldots, 9$ and all other entries equal to 0. It is known that M admits perfect state transfer from 1 to 10 at time $t_0 = \frac{\pi}{2}$, with the $(1, 10)$ entry of e^{it_0M} equal to i. Now we consider the perturbing matrix

$$M_0 = 10^{-5}\left(\frac{2}{\pi}\right) \times \begin{bmatrix} 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0.533 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.533 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{bmatrix}.$$

Setting $\hat{M} = M + M_0$, a couple of MATLAB$^{©}$ computations yield $1 - |(e^{it_0\hat{M}})_{1,10}|^2 \approx 0.02497 \times 10^{-9}$ and $\frac{2\|M_0\|_F^2}{(\pi - |\!|\!| t_0 M_0 |\!|\!|_2)^2} + |\!|\!| t_0 M_0 |\!|\!|_2^2 \approx 0.19257 \times 10^{-9}$. Therefore the actual fidelity of state transfer of the perturbed system exceeds the lower bound given by Theorem 6.2.3 approximately by 0.16760×10^{-9}.

Chapter 7

Fractional revival of threshold graphs under Laplacian dynamics

Up until now, we have been focusing on perfect state transfer, including the PST properties of different families of weighted or unweighted graphs with or without loops governed by different dynamics, and the sensitivity of the fidelity of state transfer to readout time or to edge weights when PST occurs. We have also seen examples of graphs with PGST, a generalization of PST, where the fidelity of state transfer between two fixed vertices can be made arbitrarily close to 1 by taking some specific time sequence, even though it might not attain 1.

In this chapter, we focus on fractional revival, defined in Definition 1.3.8 in terms of fidelities. Since $p_{j,k}(t) = |(U(t))_{j,k}|^2$, an equivalent definition can be stated in terms of the unitary matrix $U(t)$ directly, and we do so here. Given a system G with Hamiltonian

$\mathcal{H}$, consider the unitary matrix $U(t) = e^{it\mathcal{H}}$. If there is some time $t_2 > 0$ and two distinct vertices j and k, such that $U(t_2)e_j = \alpha e_j + \beta e_k$ for some $\alpha, \beta \in \mathbb{C}$ with $\beta \neq 0$ (since $U(t_2)$ is unitary, we know that $|\alpha|^2 + |\beta|^2 = 1$), then we say that there is *fractional revival* (FR) from j to k at time t_2 (observe that FR generalizes PST). Further, if $|\alpha| = |\beta|$, then the fractional revival is called *balanced* [26]. More generally, if there is some time $t_3 > 0$ and a proper subset S of $V(G)$, such that $|S| \geq 3$ and that for any vertex $j \in S$, $U(t_3)_{j,k} = 0$ if $k \notin S$, and the unweighted graph associated to the submatrix $U(t_3)_{[S,S]}$ is connected, then we say that there is *generalized fractional revival between vertices in* S ($U(t_3)_{[S,S]}$ is the submatrix of entries that lie in the rows and columns of $U(t_3)$ indexed by elements in S).

Fractional revival between two end vertices of a spin chain (where the underlying graph is a weighted path with loops) can also be used to transfer quantum states efficiently, and balanced fractional revival can be used to generate entangled states [14, 61]. For adjacency fractional revival to occur at the two end vertices of a weighted path with loops, the spectrum of the Hamiltonian $\mathcal{H} = A$ must take the form of a bi-lattice [42]. It is shown that spin chains with adjacency fractional revival between the end vertices can be obtained via isospectral deformations of spin chains with PST between the end vertices (note that a characterization of the spectrum of $\mathcal{H}$, or a specific edge weights set $\{w_{j,j+1} = \sqrt{j(n-j)} \,|\, j = 1, \ldots, n-1\}$, for a spin chain on n vertices to exhibit PST between the end vertices is known), and the deformation only changes the middle couplings (also the weights of the loops on the middle two vertices of the path when n is even) of the chain with PST between end vertices to get a chain with FR. In [14], a class of cubelike graphs and some weighted graphs obtained from hypercubes are found to exhibit fractional revival. In [26], some properties of adjacency fractional revival (Hamiltonian $\mathcal{H} = A$) on general graphs are studied; in particular, a characterization of fractional revival between cospectral vertices is given.

Not many graphs are known to exhibit fractional revival. Here we focus on Laplacian dynamics, and characterize the parameters of a family of graphs — threshold graphs — that admit fractional revival under Laplacian dynamics. With these threshold graphs, we can produce more graphs with Laplacian fractional revival. Recall that a *threshold graph* can be constructed from the one-vertex graph by repeatedly adding a single vertex of two possible types: an *isolated vertex*, i.e., a vertex without incident edges, or a *dominating vertex*, i.e., a vertex connected to all other vertices. A characterization of PST in threshold graphs is known (see Theorem 7.1.4 below), and consequently our results on FR in threshold graphs, which rely heavily on techniques from spectral graph theory, can be seen as an extension of that theorem.

The outline of this chapter is as follows. In Section 7.1, we review almost equitable partitions of a graph and related results about threshold graphs. In Section 7.2, we consider Laplacian fractional revival between two vertices of a graph G, where we deduce that the two vertices are strongly cospectral with respect to $L(G)$. In Section 7.3, we characterize threshold graphs that admit (generalized) Laplacian fractional revival between a subset of the vertex set. In Section 7.4, we produce more graphs with Laplacian fractional revival by making use of threshold graphs.

This chapter is based on the joint work with Kirkland [70], with myself as primary author.

7.1 Preliminaries

As described in Section 2.3.1, a partition $\pi = (C_1, \ldots, C_k)$ is an equitable partition of a graph $G = (V, E)$, if and only if,

1. the bipartite graph formed by the edges joining any two distinct cells is semi-regular (vertices in the same set of the bipartition have the same degree),
2. the induced subgraph of G on each cell C_j of π is a regular graph.

Now with a relaxation of the conditions — only requiring condition (1), we have the following notion of an almost equitable partition.

Definition 7.1.1 ([23]). *For the graph $G = (V, E)$, a partition $\pi = (C_1, \ldots, C_k)$ of its vertex set V, is called an* almost equitable partition *if $\forall j, \ell \in \{1, \ldots, k\}$ with $j \neq \ell$, the number of neighbours of a vertex $v \in C_j$ has in cell C_ℓ does not depend on the choice of v. The* generalized Laplacian matrix $L(G)^\pi$ *with respect to the almost equitable partition π is the $k \times k$ matrix such that*

$$L(G)^\pi_{j,\ell} = \begin{cases} -c_{j\ell} & \text{if } \ell \neq j \\ \sum_{r \neq j} c_{jr}, & \text{if } \ell = j, \end{cases}$$

where $c_{j\ell}$ is the number of neighbours that a vertex in cell C_j has in cell C_ℓ.

Proposition 2.3.4 shows that an equitable partition π of a graph $G = (V, E)$ can be characterized by a relation between the characteristic matrix of the partition π and the adjacency matrix $A(G)$; similarly, an almost equitable partition of a graph G can be characterized by using its characteristic matrix and the Laplacian matrix of the graph G.

Proposition 7.1.2 ([23]). *Let G be a graph, $\pi = (C_1, \ldots, C_k)$ a k-partition of $V(G)$ and P the characteristic matrix of π. Then π is an almost equitable partition if and only if there is a $k \times k$ matrix C such that*

$$L(G)P = PC$$

If π is an almost equitable k-partition, then C is the generalized Laplacian matrix $L(G)^{\pi}$.

Using two graph operations — union and join — introduced in Section 2.2, the following characterization of connected threshold graphs can be made, where we recall that K_p denotes the complete graph on p vertices and O_p denotes the empty graph on p vertices.

Proposition 7.1.3 ([69]). *Let G be a connected graph on at least two vertices. Then G is a connected threshold graph if and only if one of the following two conditions is satisfied:*

(1) there are indices $m_1, \ldots, m_{2k} \in \mathbb{N}$ with $m_1 \geq 2$ such that $G = ((((O_{m_1} \vee K_{m_2}) \cup O_{m_3}) \vee K_{m_4}) \cdots) \vee K_{m_{2k}} \equiv \Gamma(m_1, \ldots, m_{2k})$;

(2) there are indices $m_1, \ldots, m_{2k+1} \in \mathbb{N}$ with $m_1 \geq 2$ such that $G = ((((K_{m_1} \cup O_{m_2}) \vee K_{m_3}) \cup O_{m_4}) \cdots) \vee K_{m_{2k+1}} \equiv \Gamma(m_1, \ldots, m_{2k+1})$.

Order the vertices of a threshold graph $G = \Gamma(m_1, \ldots, m_{2k})$ (resp. $G = \Gamma(m_1, \ldots, m_{2k+1})$) according to the order they are added in the construction of G, that is, order the first m_1

vertices from O_{m_1} (resp. K_{m_1}), then the vertices from K_{m_2} (resp. O_{m_2}), and so on. The Laplacian PST properties of connected threshold graphs are known.

Theorem 7.1.4 ([69]). *Let G be a threshold graph. Assume $G \equiv \Gamma(m_1, \ldots, m_r)$, where r is either an even or odd integer. Then there is PST between vertex j and k at time $t \in [0, \pi]$ if and only if $\{j, k\} = \{1, 2\}$ and in addition: $t = \pi/2$; $m_1 = 2$; $m_2 \equiv 2 \pmod 4$, and $m_\ell \equiv 0 \pmod 4$ for $\ell \geq 3$.*

In this chapter, subscripts denoting the sizes of matrices and vectors will be suppressed when they are clear from the context. Eigenvalues are labelled so that the smallest eigenvalue 0 is denoted by λ_0.

7.2 Laplacian fractional revival between two vertices

Assume that G is a graph on n vertices and that it admits Laplacian fractional revival from vertex u to vertex v at time t. Without loss of generality, assume that vertices u and v are labelled 1 and 2, respectively. Then $U(t) = e^{itL(G)} = \begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix}$ for some complex symmetric unitary matrices U_1 of size 2×2 and U_2 of size $(n-2) \times (n-2)$, and the union of the spectrum of U_1 and the spectrum of U_2 gives the spectrum of $U(t)$. Denote the (j, ℓ) entry of U_1 by $U_{j,\ell}$, then for $j = 1, 2$, $e^{itL(G)} e_j = U_{1,j} e_1 + U_{2,j} e_2$. Now assume that the spectral decomposition of $L(G)$ is $L(G) = \sum_{r=0}^{q} \theta_r E_r$ with $\theta_0 = 0$. Then $e^{itL(G)} = \sum_{r=0}^{q} e^{it\theta_r} E_r$ by Theorem 2.1.2, and $e^{itL(G)} e_u = \sum_{r=0}^{q} e^{it\theta_r} E_r e_u$ for any vertex u of G. Therefore $\sum_{r=0}^{q} e^{it\theta_r} E_r e_j = e^{itL(G)} e_j = U_{1,j} e_1 + U_{2,j} e_2$ for $j = 1, 2$. Premultiplying

E_r on both sides of the equation, combined with the facts that $E_r E_\ell = \delta_{r,\ell} E_r$, and that $e^{itL(G)}$ and E_r commute, gives $e^{it\theta_r} E_r e_j = U_{1,j} E_r e_1 + U_{2,j} E_r e_2$ for $j = 1, 2$. Putting the equations for $j = 1$ and $j = 2$ together gives $[E_r e_1 , E_r e_2](U_1 - e^{it\theta_r} I_2) = 0_{n,2}$ for $r = 0, 1, \dots, q$. Therefore if $C_r = [E_r e_1 , E_r e_2] \neq 0_{n,2}$, then $e^{it\theta_r}$ is an eigenvalue of U_1, and that any nonzero row of C_r is a real left eigenvector of U_1 associated to the eigenvalue $e^{it\theta_r}$. In particular, for $\theta_0 = 0$, $C_0 = \frac{1}{n} J_{n,2} \neq 0_{n,2}$ (as $E_0 = \frac{1}{n} J_n$), and therefore $e^{it\theta_0} = e^{it0} = 1$ is an eigenvalue of U_1. Furthermore, 1 is a simple eigenvalue of U_1, since the only 2×2 diagonalizable matrix that has 1 as a multiple eigenvalue is the identity matrix I_2.

Note that for a complex symmetric matrix, each of its real eigenvectors is a left eigenvector at the same time, and the real eigenvectors associated to distinct eigenvalues are orthogonal. To see this, assume that U is a complex symmetric matrix, with a real eigenvector x associated to λ, and a real eigenvector y associated to $\mu \neq \lambda$. Taking the transpose of $Ux = \lambda x$ gives $x^T U = x^T U^T = (Ux)^T = \lambda x^T$, that is to say, x is also a left eigenvector of U. From $\lambda x^T y = (x^T U)y = x^T (Uy) = \mu x^T y$ and $\lambda \neq \mu$, we conclude that $x^T y = 0$, i.e., x and y are orthogonal to each other.

Now consider any eigenvalue θ_r of $L(G)$ such that $e^{it\theta_r}$ is an eigenvalue of U_1 (therefore any nonzero row of $C_r = [E_r e_1 , E_r e_2]$ is a left eigenvector of U_1 associated to $e^{it\theta_r}$). If $e^{it\theta_r} \neq 1$, from the facts that U_1 is symmetric, E_r is a real matrix for $r = 0, 1, \dots, q$, and that $\mathbf{1}_2$ is an eigenvector of U_1 associated to the eigenvalue 0, we know that $C_r \mathbf{1}_2 = [E_r e_1 , E_r e_2]\mathbf{1}_2 = \mathbf{0}_n$, i.e., $E_r e_1 + E_r e_2 = \mathbf{0}_n$. Since 1 is a simple eigenvalue of U_1, for each $r \in \{0, 1, \dots, q\}$ such that $e^{it\theta_r} = 1$, all the rows of C_r are scalar multiples of $\mathbf{1}_2^T$. That is to say, $[E_r e_1\,, E_r e_2] = [E_r e_1\,, E_r e_1]$, or $E_r e_1 = E_r e_2$. The following theorem summarizes these observations.

Theorem 7.2.1. *If a weighted graph G admits Laplacian fractional revival between two vertices u and v at time t, then the two vertices u and v are strongly cospectral with respect to the Laplacian matrix $L(G)$. That is, if the spectral decomposition of $L(G)$ is $L(G) = \sum_r \theta_r E_r$, then for each r, either $E_r e_u = E_r e_v$ (if $\frac{t\theta_r}{2\pi} \in \mathbb{Z}$) or $E_r e_u = -E_r e_v$ (if $\frac{t\theta_r}{2\pi} \notin \mathbb{Z}$) holds.*

While preparing [70], we learned that Chan and Teitelbaum [27] have also proved the necessity of strong cospectrality of the two vertices for Laplacian FR.

Remark 7.2.2. If a weighted G admits generalized Laplacian fractional revival between $m \geq 3$ vertices at time t, then 1 is not necessary a simple eigenvalue of U_1 — the submatrix of $U(t) = e^{itL(G)}$ corresponding to the m vertices, but if it is, then with a similar argument as above, we have the following.

Assume that G is a weighted graph that admits generalized Laplacian fractional revival between vertices in $S = \{1, 2, \dots, m\} \subset V(G)$ at time t, and that $U_1 = U(t)_{[S,S]} = (e^{itL(G)})_{[S,S]}$ has 1 as a simple eigenvalue. Let $L(G) = \sum_{r=0}^{q} \theta_r E_r$ be the spectral decomposition of the Laplacian matrix $L(G)$. Then for each $r = 0, 1, \dots, q$, the vectors $E_r e_1,\ E_r e_2,\ \cdots,\ E_r e_m$ are linearly dependent, and either

$$E_r e_1 = E_r e_2 = \cdots = E_r e_m \text{ if } e^{it\theta_r} = 1, \text{ or} \tag{7.1}$$

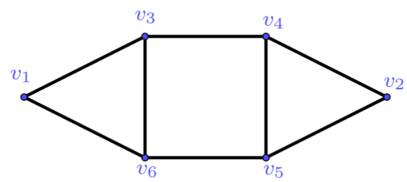


Figure 7.1: A graph with a vertex involved in fractional revival and generalized fractional revival at different time

$$E_r e_1 + E_r e_2 + \cdots + E_r e_m = \mathbf{0} \text{ if } e^{it\theta_r} \neq 1. \tag{7.2}$$

Example 7.2.3. Let G be the graph as shown in Figure 7.1, and write the spectral decomposition of its Laplacian as $L(G) = \sum_{r=0}^{4} \theta_r E_r$, with $\theta_0 = 0$, $\theta_1 = 1$, $\theta_2 = 3$, $\theta_3 = 4$, and $\theta_4 = 5$. There is Laplacian fractional revival between vertices v_1 and v_2, and generalized fractional revival between vertices $\{v_3, v_4, v_5, v_6\}$ at time $\frac{2\pi}{3}$. Direct observation shows that v_1 and v_2 are strongly cospectral with respect to $L(G)$: $E_r e_1 = E_r e_2$ for $r = 0, 2$, $E_r e_1 = -E_r e_2$ for $r = 1, 3$, and $E_4 e_1 = E_4 e_2 = \mathbf{0}_6$, which is in accordance with Theorem 7.2.1. There is also generalized Laplacian fractional revival between vertices $\{v_1, v_4, v_5\}$, and between vertices $\{v_2, v_3, v_6\}$ at time π. Since 1 is a simple eigenvalue of $U_1 = U(\pi)_{[\{1,4,5\},\{1,4,5\}]}$, Remark 7.2.2 implies that $E_r e_1 = E_r e_4 = E_r e_5$ for $r = 0, 3$ ($e^{i\pi\theta_r} = 1$) and that $E_r e_1 + E_r e_4 + E_r e_5 = \mathbf{0}$ for $r = 1, 2, 4$ (since $e^{i\pi\theta_r} \neq 1$), which can be confirmed by checking the orthogonal projection matrices E_r directly.

7.3 Laplacian fractional revival in threshold graphs

We will only give detailed consideration to connected threshold graphs of the form $\Gamma(m_1, m_2, \ldots, m_{2k})$ in this section; note that similar results hold for the connected threshold graphs $\Gamma(m_1, m_2, \ldots, m_{2k}, m_{2k+1})$, and we state them without proof.

As shown by Kirkland and Severini [69], the Laplacian eigenvalues of the threshold graph $\Gamma(m_1, m_2, \ldots, m_{2k})$ are:

$$\begin{aligned} \lambda_0 &= 0, \\ \lambda_j &= m_{j+1} + m_{j+3} + \cdots + m_{2k} \text{ for any odd integer } j \in \{1, \ldots, 2k\}, \text{ and} \\ \lambda_j &= \sigma_j + m_{j+2} + \cdots + m_{2k} \text{ for any even integer } j \in \{1, \ldots, 2k\}, \end{aligned} \tag{7.3}$$

where $\sigma_j := m_1 + m_2 + \cdots + m_j$ for $j = 1, 2, \ldots, 2k$. The multiplicity of λ_j is

$$\begin{cases} 1, & \text{if } j = 0 \\ m_1 - 1, & \text{if } j = 1 \\ m_j, & \text{otherwise.} \end{cases}$$

The orthogonal idempotents for $L(G)$ corresponding to $\lambda_0 = 0$, $\lambda = \lambda_1$ and $\lambda = \lambda_j$ for $j = 2, 3, \ldots, 2k$ are: $E_0 = \frac{1}{\sigma_{2k}} J_{\sigma_{2k}}$,

$$\begin{aligned} E_1 &= \begin{bmatrix} I_{m_1} - \frac{1}{m_1} J_{m_1} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}, \text{ and} \\ E_j &= \begin{bmatrix} \frac{m_j}{\sigma_{j-1}\sigma_j} J_{\sigma_{j-1}} & -\frac{1}{\sigma_j} J_{\sigma_{j-1}, m_j} & 0_{\sigma_{j-1}, \sigma_{2k}-\sigma_j} \\ -\frac{1}{\sigma_j} J_{m_j, \sigma_{j-1}} & I_{m_j} - \frac{1}{\sigma_j} J_{m_j} & 0_{m_j, \sigma_{2k}-\sigma_j} \\ 0_{\sigma_{2k}-\sigma_j, \sigma_{j-1}} & 0_{\sigma_{2k}-\sigma_j, m_j} & 0_{\sigma_{2k}-\sigma_j, \sigma_{2k}-\sigma_j} \end{bmatrix}, \text{respectively.} \end{aligned}$$

We partition the vertex set of $\Gamma(m_1, \ldots, m_{2k})$ according to the indices $m_1, m_2, \ldots, m_{2k}$; denote the corresponding cells by $C_1, C_2, \ldots, C_{2k}$, and denote the partition by π.

Lemma 7.3.1. *If $G = \Gamma(m_1, \ldots, m_{2k})$ admits Laplacian fractional revival between two vertices u and v, then u and v belong to the same cells of the partition π.*

Proof. From Theorem 7.2.1 we know that if there is Laplacian fractional revival between two vertices u and v of $G = \Gamma(m_1, \ldots, m_{2k})$, then the two vertices are strongly cospectral with respect to $L(G)$. Assume that $u \in C_j$, $v \in C_\ell$, $j < \ell$, and that u is the s-th entry of cell C_j. Then $E_j e_v = \mathbf{0}_{\sigma_{2k}}$ and for $e_s \in \mathbb{R}^{m_j}$, $E_j e_u = \left[\begin{array}{c|c} e_s^T - \frac{1}{m_1}\mathbf{1}_{m_1}^T & \mathbf{0}_{\sigma_{2k}-m_1}^T \end{array}\right]^T$ if $j = 1$; $E_j e_u = \left[\begin{array}{c|c|c} -\frac{1}{\sigma_j}\mathbf{1}_{\sigma_{j-1}}^T & e_s^T - \frac{1}{\sigma_j}\mathbf{1}_{m_j}^T & \mathbf{0}_{\sigma_{2k}-\sigma_j}^T \end{array}\right]^T$ if $j > 1$. In either case, u and v are not strongly cospectral with respect to $L(G)$. Therefore u and v must be in the same cell of the partition π. $\square$

Lemma 7.3.2. *If $G = \Gamma(m_1, \ldots, m_{2k})$ admits Laplacian fractional revival between two vertices u and v, then $\{u, v\} = \{1, 2\}$ and $m_1 = 2$.*

Proof. From Lemma 7.3.1 we know that vertices u and v are in the same cell of π; assume $u, v \in C_j$, with u being the s-th vertex in C_j, and v the r-th vertex in C_j. Let $\sigma_0 = 0$, then $E_j e_u = \left[\begin{array}{c|c|c} -\frac{1}{\sigma_j}\mathbf{1}_{\sigma_{j-1}}^T & (e_s - \frac{1}{\sigma_j}\mathbf{1}_{m_j})^T & \mathbf{0}_{\sigma_{2k}-\sigma_j}^T \end{array}\right]^T$ and $E_j e_v = \left[\begin{array}{c|c|c} -\frac{1}{\sigma_j}\mathbf{1}_{\sigma_{j-1}}^T & (e_r - \frac{1}{\sigma_j}\mathbf{1}_{m_j})^T & \mathbf{0}_{\sigma_{2k}-\sigma_j}^T \end{array}\right]^T$, where $e_s, e_r \in \mathbb{R}^{m_j}$. By Theorem 7.2.1, Laplacian fractional revival between u and v implies $E_j e_u = \pm E_j e_v$, which is possible only if $j = 1$ and $\sigma_1 = m_1 = 2$. $\square$

Now we are going to characterize the parameters m_j such that Laplacian fractional revival occurs between vertices 1 and 2 in the graph $G = \Gamma(m_1, \ldots, m_{2k})$ by using the spectral decomposition of $L(G)$ shown at the beginning of this section. Since all the eigenvalues of $L(G)$ are integers, we know that G is Laplacian periodic at all vertices at time 2π, i.e. $e^{2\pi i L(G)}$ is a scalar multiple of the identity matrix (in fact it is the identity matrix here). In the following we will not consider this case, or any time larger than 2π.

Theorem 7.3.3. *The threshold graph $G = \Gamma(m_1, \dots, m_{2k})$ admits Laplacian fractional revival between two vertices u and v at time t if and only if*

1. $\{u, v\} = \{1, 2\}$ *and* $m_1 = 2$, *and*

2. (a) $m_1 \frac{t}{\pi} = 2\frac{t}{\pi} \notin \mathbb{Z}$,

   (b) $(m_1 + m_2)\frac{t}{2\pi}, m_j \frac{t}{2\pi} \in \mathbb{Z}$ *for* $j = 3, \dots, 2k$.

Proof. Assume that there is Laplacian fractional revival between vertices u and v at time

$t > 0$. Then Lemmas 7.3.1 and 7.3.2 imply that $1.)$ holds. Using the spectral decomposition of $L(G)$ we have

$$\begin{aligned}
(e^{itL(G)})_{1,1} &= e^{it\lambda_1}(1-\tfrac{1}{2}) + e^{it\lambda_2}(\tfrac{m_2}{\sigma_1\sigma_2}) + e^{it\lambda_3}(\tfrac{m_3}{\sigma_2\sigma_3}) + \cdots \\
&\quad + e^{it\lambda_{2k-1}}(\tfrac{m_{2k-1}}{\sigma_{2k-2}\sigma_{2k-1}}) + e^{it\lambda_{2k}}(\tfrac{m_{2k}}{\sigma_{2k-1}\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}} \\
&= e^{it\lambda_1}(1-\tfrac{1}{2}) + e^{it\lambda_2}(\tfrac{1}{\sigma_1} - \tfrac{1}{\sigma_2}) + e^{it\lambda_3}(\tfrac{1}{\sigma_2} - \tfrac{1}{\sigma_3}) + \cdots \\
&\quad + e^{it\lambda_{2k-1}}(\tfrac{1}{\sigma_{2k-2}} - \tfrac{1}{\sigma_{2k-1}}) + e^{it\lambda_{2k}}(\tfrac{1}{\sigma_{2k-1}} - \tfrac{1}{\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}}, \\
(e^{itL(G)})_{1,2} &= e^{it\lambda_1}(-\tfrac{1}{2}) + e^{it\lambda_2}(\tfrac{m_2}{\sigma_1\sigma_2}) + e^{it\lambda_3}(\tfrac{m_3}{\sigma_2\sigma_3}) + \cdots \\
&\quad + e^{it\lambda_{2k-1}}(\tfrac{m_{2k-1}}{\sigma_{2k-2}\sigma_{2k-1}}) + e^{it\lambda_{2k}}(\tfrac{m_{2k}}{\sigma_{2k-1}\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}} \qquad (7.4) \\
&= e^{it\lambda_1}(-\tfrac{1}{2}) + e^{it\lambda_2}(\tfrac{1}{\sigma_1} - \tfrac{1}{\sigma_2}) + e^{it\lambda_3}(\tfrac{1}{\sigma_2} - \tfrac{1}{\sigma_3}) + \cdots \\
&\quad + e^{it\lambda_{2k-1}}(\tfrac{1}{\sigma_{2k-2}} - \tfrac{1}{\sigma_{2k-1}}) + e^{it\lambda_{2k}}(\tfrac{1}{\sigma_{2k-1}} - \tfrac{1}{\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}}, \\
(e^{itL(G)})_{1,w} &= e^{it\lambda_j}(-\tfrac{1}{\sigma_j}) + e^{it\lambda_{j+1}}(\tfrac{m_{j+1}}{\sigma_j\sigma_{j+1}}) + \cdots + e^{it\lambda_{2k}}(\tfrac{m_{2k}}{\sigma_{2k-1}\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}} \\
&= e^{it\lambda_j}(-\tfrac{1}{\sigma_j}) + e^{it\lambda_{j+1}}(\tfrac{1}{\sigma_j} - \tfrac{1}{\sigma_{j+1}}) + \cdots \\
&\quad + e^{it\lambda_{2k}}(\tfrac{1}{\sigma_{2k-1}} - \tfrac{1}{\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}} \quad \text{for } w \in C_j \text{with } j = 2, \ldots, 2k.
\end{aligned}$$

Since $(e^{itL(G)})_{1,w} = 0$ for $w \neq 1, 2$, then considering $w \in C_{2k}$, $w \in C_{2k-1}$, $\ldots, w \in C_3, w \in C_2$, we find that $t\sigma_{2k}$, tm_{2k}, $t(\sigma_{2k-2} + m_{2k})$, $\ldots$, $t(m_4 + m_6 + \ldots + m_{2k})$, and $t(\sigma_2 + m_4 + \ldots + m_{2k})$ are all even integer multiples of π, which is equivalent to the fact that tm_{2k}, tm_{2k-1}, tm_{2k-2}, $\ldots$, tm_3, and $t\sigma_2$ are all even integer multiples of π. In this case, (7.4) gives

$$(e^{itL(G)})_{1,1} = \frac{1}{2}e^{itm_2} + \frac{1}{2}, \text{and } (e^{itL(G)})_{1,2} = -\frac{1}{2}e^{itm_2} + \frac{1}{2}. \qquad (7.5)$$

Hence, if in addition,

- tm_2 (and therefore $tm_1 = 2t$) is an even integer multiple of π, then the graph G is periodic at vertex 1 (and vertex 2);

- tm_2 (and therefore $tm_1 = 2t$) is an odd integer multiple of π, then the graph G admits Laplacian perfect state transfer between vertex 1 and 2;

- tm_2 (and therefore $tm_1 = 2t$) is not an integer multiple of π, then the graph G admits Laplacian fractional revival between vertex 1 and 2.

Therefore the conditions are necessary. It is straightforward to show that the conditions are sufficient. $\square$

Similarly to the above, the following can be proved.

Remark 7.3.4. The threshold graph $G = \Gamma(m_1, \ldots, m_{2k}, m_{2k+1})$ admits Laplacian fractional revival between two vertices u and v at time t if and only if

1. $\{u, v\} = \{1, 2\}$ and $m_1 = 2$, and
2. (a) $m_1 \frac{t}{\pi} = 2\frac{t}{\pi} \notin \mathbb{Z}$,

   (b) $(m_1 + m_2)\frac{t}{2\pi}, m_j \frac{t}{2\pi} \in \mathbb{Z}$ for $j = 3, \ldots, 2k, 2k+1$.

Corollary 7.3.5. *There is balanced Laplacian fractional revival between vertices u and v in the threshold graph $G = \Gamma(m_1, \ldots, m_{2k})$ at time t if and only if*

1. *$m_1 = 2$ with $\{u, v\} = \{1, 2\}$,*
2. *$t = \frac{2\ell+1}{4}\pi$ for some non-negative integer ℓ,*

3. *$m_2 = \frac{2(2s+1)}{2\ell+1}$, for the same integer ℓ as in 2.) above, and for a non-negative integer s of distinct parity from ℓ such that $(2\ell+1)|(2s+1)$ (in fact when this is true, then necessarily $\frac{2s+1}{2\ell+1} \equiv 3 \pmod 4$), and*

4. *$m_j \equiv 0 \pmod 8$ for $j = 3, \ldots, 2k$.*

Proof. From Theorem 7.3.3, we know that if balanced fractional revival takes place in G between vertices u and v, then it is between vertices 1 and 2. In this case, Theorem 7.3.3 and equation (7.5) imply that $m_1 = 2$, $\cos(m_2 t) = 0$, and $t(m_1 + m_2), tm_3, \ldots, tm_{2k}$ are all even integer multiples of π. Therefore $tm_2 = \frac{2s+1}{2}\pi$ for some integer s. Since $t(m_1 + m_2)$ is an even integer multiple of π, $2t = \frac{2\ell+1}{2}\pi$ for some integer ℓ, where ℓ has different parity than s. Hence $t = \frac{2\ell+1}{4}\pi$ and $m_2 = \frac{2(2s+1)}{2\ell+1}$ for integers s and ℓ with distinct parity. Combining with the fact that tm_j is an even integer multiple of π for $j = 3, \ldots, 2k$, we find that $m_j \equiv 0 \pmod 8$ for $j \geq 3$.

Conversely, if $m_j \equiv 0 \pmod 8$ for $j \geq 3$, and $t = \frac{2\ell+1}{4}\pi$ for some integer ℓ, then $m_j t = m_j \frac{2\ell+1}{4}\pi$ is an even integer multiple of π for $j \geq 3$. Furthermore, if $m_2 = \frac{2(2s+1)}{2\ell+1}$ for an integer s of different parity than ℓ such that $(2\ell+1)|(2s+1)$, then $(m_1 + m_2)t = (s+\ell+1)\pi$ is an even integer multiple of π, and $\cos(m_2 t) = \cos(\frac{2s+1}{2}\pi) = 0$. Again from Theorem 7.3.3 and equation (7.5), we know that there is balanced fractional revival in G between vertex 1 and 2 at time t. $\square$

Remark 7.3.6. There is balanced Laplacian fractional revival between vertices u and v in the threshold graph $G = \Gamma(m_1, \ldots, m_{2k}, m_{2k+1})$ at time t, if and only if

1. $m_1 = 2$ with $\{u, v\} = \{1, 2\}$,

2. $t = \frac{2\ell+1}{4}\pi$ for some non-negative integer ℓ,

3. $m_2 = \frac{2(2s+1)}{2\ell+1}$, for the same integer ℓ as in 2.), and for a non-negative integer s of distinct parity from ℓ such that $(2\ell + 1)|(2s + 1)$ (in fact when this is true, then necessarily $\frac{2s+1}{2\ell+1} \equiv 3 \pmod 4$), and

4. $m_j \equiv 0 \pmod 8$ for $j = 3, \ldots, 2k, 2k + 1$.

Remark 7.3.7. Since if there is PST between vertices u and v, then u and v are strongly cospectral [45], the proof of Theorem 7.3.3 can be used to prove Theorem 7.1.4: the second of the three cases in the proof gives us Theorem 7.1.4.

Now we address generalized Laplacian fractional revival within some subset of vertices in threshold graphs.

Theorem 7.3.8. *Consider the threshold graph $G = \Gamma(m_1, \ldots, m_{2k})$, and let $C_\ell, \ell = 1, \ldots, 2k$ denote the cells of the partition π of $V(G)$ according to the parameters $m_\ell, \ell = 1, \ldots, 2k$. Then G admits generalized Laplacian fractional revival between vertices in $S \subset V(G)$ at some time $t > 0$ if and only if, for some integer $j < 2k$, tm_{2k}, tm_{2k-1}, $\ldots$, tm_{j+2} and $t\sigma_{j+1}$ are all even integer multiples of π, while tm_{j+1} is not. In this case, $S = C_1 \cup \cdots \cup C_j$, and G is periodic at all vertices in the cells $C_{j+1}, \ldots, C_{2k}$.*

Proof. Assume G admits generalized Laplacian fractional revival between vertices in S at time t, with j being the largest number such that $S \cap C_j \neq \emptyset$. Let u be any vertex in

$S \cap C_j$. Now for any $w \in C_\ell$, with $\ell = j+1, \ldots, 2k$,

$$\begin{aligned}(e^{itL(G)})_{u,w} &= e^{it\lambda_\ell}(-\tfrac{1}{\sigma_\ell}) + e^{it\lambda_{\ell+1}}(\tfrac{m_{\ell+1}}{\sigma_\ell\sigma_{\ell+1}}) + \cdots + e^{it\lambda_{2k}}(\tfrac{m_{2k}}{\sigma_{2k-1}\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}} \\ &= e^{it\lambda_\ell}(-\tfrac{1}{\sigma_\ell}) + e^{it\lambda_{\ell+1}}(\tfrac{1}{\sigma_\ell} - \tfrac{1}{\sigma_{\ell+1}}) + \cdots + e^{it\lambda_{2k}}(\tfrac{1}{\sigma_{2k-1}} - \tfrac{1}{\sigma_{2k}}) + \tfrac{1}{\sigma_{2k}};\end{aligned}$$

for any $v \in C_1 \cup C_2 \cup \cdots \cup C_j$ with $v \neq u$,

$$(e^{itL(G)})_{u,v} = e^{it\lambda_j}(-\frac{1}{\sigma_j}) + e^{it\lambda_{j+1}}(\frac{1}{\sigma_j} - \frac{1}{\sigma_{j+1}}) + \cdots + e^{it\lambda_{2k}}(\frac{1}{\sigma_{2k-1}} - \frac{1}{\sigma_{2k}}) + \frac{1}{\sigma_{2k}},$$

and for any $x \in C_\ell$, with $\ell = 1, \ldots, 2k$,

$$(e^{itL(G)})_{x,x} = e^{it\lambda_\ell}(1 - \frac{1}{\sigma_\ell}) + e^{it\lambda_{\ell+1}}(\frac{1}{\sigma_\ell} - \frac{1}{\sigma_{\ell+1}}) + \cdots + e^{it\lambda_{2k}}(\frac{1}{\sigma_{2k-1}} - \frac{1}{\sigma_{2k}}) + \frac{1}{\sigma_{2k}}.$$

Since $(e^{itL(G)})_{u,w} = 0$ for $w \in C_{2k}, C_{2k-1}, \ldots, C_{j+1}$, we find that

$$\frac{tm_{2k}}{2\pi}, \frac{tm_{2k-1}}{2\pi}, \ldots, \frac{tm_{j+2}}{2\pi}, \frac{t\sigma_{j+1}}{2\pi} \in \mathbb{Z}. \tag{7.6}$$

In this case, for $w \in C_{j+1} \cup \ldots \cup C_{2k}$,

$$\begin{aligned}(e^{itL(G)})_{w,w} &= 1, \\ (e^{itL(G)})_{u,u} &= e^{it\lambda_j}\left(1 - \frac{1}{\sigma_j}\right) + \frac{1}{\sigma_j}, \text{ and} \\ (e^{itL(G)})_{u,v} &= e^{it\lambda_j}\left(-\frac{1}{\sigma_j}\right) + \frac{1}{\sigma_j} \text{ for } v \in C_1 \cup \ldots \cup C_j \text{ and } v \neq u.\end{aligned} \tag{7.7}$$

Therefore G is periodic at any vertex $w \in C_{j+1} \cup \ldots \cup C_{2k}$. The fact that u is involved in generalized Laplacian fractional revival implies that $|(e^{itL(G)})_{u,u}| \neq 1$. Combining with (7.7) and (7.6), we find that $\frac{tm_{j+1}}{2\pi} \notin \mathbb{Z}$ (no matter j is even or odd), and therefore $(e^{itL(G)})_{u,v} \neq 0$ for any $v \in C_1, \ldots, C_{j-1}, C_j$ (if $(e^{itL(G)})_{u,u} = 0$, then $\sigma_j = 2$, $j = 1$ and there is Laplacian PST between vertices 1 and 2, which is not the case we are considering).

Hence $S = C_1 \cup \ldots \cup C_j$ and the conditions are necessary. The other direction follows readily. □

Remark 7.3.9. For the threshold graph $G = \Gamma(m_1, \ldots, m_{2k}, m_{2k+1})$, let $C_\ell, \ell = 1, \ldots, 2k+1$ denote the cells of the partition π of $V(G)$ according to the parameters $m_\ell, \ell = 1, \ldots, 2k+1$. Then G admits generalized Laplacian fractional revival between vertices in $S \subset V(G)$ at some time $t > 0$ if and only if, for some integer $j < 2k+1$, tm_{2k+1}, tm_{2k}, tm_{2k-1}, $\ldots$, tm_{j+2} and $t\sigma_{j+1}$ are all even integer multiples of π, while tm_{j+1} is not. In this case, $S = C_1 \cup \cdots \cup C_j$, and G is Laplacian periodic at all vertices in the cells $C_{j+1}, \ldots, C_{2k}, C_{2k+1}$.

Example 7.3.10. Consider the threshold graph $G = \Gamma(2, 2, 2, 2, 4, 4)$. Direction computation (by the spectral decomposition as in Theorem 2.1.2 and Remark 2.1.3) shows that there is generalized Laplacian fractional revival between all vertices in the set $S = \{1, 2, \ldots, 6\}$ at $t = \pi/2$. The result is in correspondence with Theorem 7.3.8, since $tm_5 = tm_6$ and $t\sigma_4 = 8t$ are all even integer multiples of π, while $tm_4 = \pi$ is not. Similarly $\Gamma(3, 1, 4)$ admits Laplacian fractional revival between the first 4 vertices at time $t = \frac{\pi}{4}$, and $\Gamma(2, 2, 6, 2, 4, 4)$ admits Laplacian fractional revival between the first 10 vertices at time $t = \frac{\pi}{2}$.

Remark 7.3.11. Note that Theorem 7.3.8 implies Theorem 7.3.3, but the strong cospectrality of the two vertices involved in Laplacian fractional revival makes the proof more clear as shown in Theorem 7.3.3.

7.4 Constructing graphs with Laplacian fractional revival

More graphs with Laplacian fractional revival can be obtained from those threshold graphs that admit Laplacian fractional revival. To construct such graphs, we make use of almost equitable partitions of a graph. First note that apart from Proposition 7.1.2, there are other equivalent characterizations of an almost equitable partition of a graph. The proof is essentially the same as that for the characterization of equitable partitions as in Theorem 2.3.5, but we include it for completeness.

Proposition 7.4.1. *Suppose that $\pi = (C_1, \ldots, C_k)$ is a partition of the vertices of the graph G, and that $\hat{P}$ is its normalized characteristic matrix. Then the following are equivalent:*

(a) π is almost equitable.

(b) The column space of $\hat{P}$ is $L(G)$-invariant.

(c) There is a $k \times k$ matrix B such that $L(G)\hat{P} = \hat{P}B$.

(d) $L(G)$ and $\hat{P}\hat{P}^T$ commute.

Proof. Assume P is the characteristic matrix of the partition π. From Theorem 7.1.2 we know that π is an almost equitable partition if and only if $L(G)P = PL(G)^{\pi}$, i.e., the column space of P is $L(G)$-invariant. Since P and $\hat{P}$ have the same column space, it follows that (a) and (b) are equivalent.

Since (c) is an equivalent way to say that the column space of $\hat{P}$ is $L(G)$-invariant, (b) and (c) are equivalent. Furthermore, $L(G)\hat{P} = \hat{P}B$ implies that $\hat{P}^T L(G)\hat{P} = \hat{P}^T\hat{P}B =$

$I_k B = B$, from which we see that the matrix B in (c) is symmetric.

Now if (c) is true, and using the fact that B is symmetric, we have $L(G)\hat{P}\hat{P}^T = \hat{P}B\hat{P}^T = \hat{P}(\hat{P}B)^T = \hat{P}(L(G)\hat{P})^T = \hat{P}\hat{P}^T L(G)$, and therefore (c) implies (d).

To prove that (d) implies (b), we note that if $L(G)$ commutes with a matrix S, then the column space of S is $L(G)$-invariant. Combined with the fact that $\hat{P}\hat{P}^T$ and $\hat{P}$ have the same column space, we get the desired result. $\square$

If a graph G_1 admits an equitable partition π_1 with vertices u and v being singletons, then as shown in Theorem 2.3.6, $(e^{itA(G_1)})_{u,v} = (e^{itA(\widehat{G_1/\pi_1})})_{\{u\},\{v\}}$, where $A(\widehat{G_1/\pi_1}) = \hat{P}^T A(G_1)\hat{P}$, with rows and columns indexed by the cells of the partition π_1, and it is the adjacency matrix of the symmetrized quotient graph of G with respect to π_1. Now if a graph G admits an almost equitable partition, then a parallel result holds between $L(G)$ and $\widehat{L(G)^\pi}$ with exactly the same argument, where $\widehat{L(G)^\pi} = \hat{P}^T L(G)\hat{P}$ (note that in general, $\widehat{L(G)^\pi}$ is not the Laplacian matrix of a weighted graph without loops, that is, generally $\widehat{L(G)^\pi}\mathbf{1} \neq \mathbf{0}$).

Theorem 7.4.2. *Let $G = (V, E)$ be a graph with an almost equitable partition π, where two distinct vertices j and ℓ belong to singleton cells. Let $L(G)$ denote its Laplacian matrix. Let u, v be either j or ℓ (introduced to include the four equations about $\{j, j\}$, $\{j, k\}$, $\{k, j\}$, and $\{k, k\}$ in one, as the following). Then for any time t,*

$$(e^{itL(G)})_{u,v} = (e^{it\widehat{L(G)^\pi}})_{\{u\},\{v\}},$$

where $\{u\}$ and $\{v\}$ are the corresponding singleton cells of π, and the cells of π are *used to index rows and columns of $\widehat{L(G)^\pi}$. Therefore, the system with Hamiltonian $L(G)$ admits fractional revival (resp. perfect state transfer) from j to ℓ at time t if and only if the system with Hamiltonian $\widehat{L(G)^\pi} = \hat{P}^T L(G) \hat{P}$ admits fractional revival (resp. perfect state transfer) from $\{j\}$ to $\{\ell\}$ at time t.*

The above result was used in an example in [2]. Similarly, if a graph G admits generalized Laplacian fractional revival between vertices $u_1, \dots, u_m$ at time t and G has an almost equitable partition π such that $u_1 \dots, u_m$ are all singletons, then the system with Hamiltonian $\widehat{L(G)^\pi}$ admits generalized Laplacian fractional revival between vertices $\{u_1\}, \dots, \{u_m\}$ at time t. Now we can construct more graphs with (generalized) Laplacian fractional revival (resp. Laplacian perfect state transfer) from some given graphs.

Corollary 7.4.3. *Suppose that a graph $G = (V, E)$ has an almost equitable partition π of V, with vertices u and v belonging to singleton cells. If there is Laplacian fractional revival (resp. Laplacian perfect state transfer, Laplacian pretty good state transfer) from u to v in G, then for any graph Y obtained from G by adding or deleting any collection of edges within the cells of π, Y also admits Laplacian fractional revival (resp. Laplacian perfect state transfer, Laplacian pretty good state transfer) from u to v.*

Proof. The almost equitable partition π of the vertex set of G is also an almost equitable partition of $V(Y)$. From the fact that $\widehat{L(Y)^\pi} = \hat{P}^T L(Y) \hat{P} = \hat{P}^T L(G) \hat{P} = \widehat{L(G)^\pi}$ and Theorem 7.4.2, the result follows. $\square$

Remark 7.4.4. The partition π of a threshold graph according to the parameters m_j is an (almost) equitable partition, and so is any refinement of this partition. In particular, for a threshold graph G that admits Laplacian fractional revival at time t, partitioning the cell $C_1 = \{1,2\}$ of π into two smaller cells $C_{1,1} = \{1\}$ and $C_{1,2} = \{2\}$ and keeping all the other cells unchanged, results in the partition π', that is still an almost equitable partition of $V(G)$, but now the two vertices involved in Laplacian fractional revival are singletons. Therefore, we can produce more graphs with Laplacian fractional revival from the threshold graph G by adding or deleting edges inside the cells of the partition π' of $V(G)$. Similarly, if a threshold graph G admits generalized Laplacian fractional revival at time t between vertices $\{1,\dots,\ell\} = C_1 \cup \cdots \cup C_j$, where $C_1,\dots,C_{2k}$ (C_{2k+1}) are the cells of the partition π, then the refinement π'' of π, which partitions $C_1 \cup \cdots \cup C_j$ into singletons as $\{1\},\dots,\{\ell\}$ and keeps all the other cells of π unchanged, is still an almost equitable partition of $V(G)$, but with all the vertices involved in the revival being singletons. Again, adding or deleting edges inside the cells of the partition π'' results in graphs that admit generalized Laplacian fractional revival between vertices $\{1,\dots,\ell\}$ at time t.

Example 7.4.5. For any threshold graph $G = \Gamma(m_1,\dots,m_{2k})$ with Laplacian fractional revival (resp. Laplacian PST, Laplacian PGST), and for any odd integer $p > 1$, even integer $q \geq 2$, the graph Y obtained from G by adding edges in the induced subgraph O_{m_p} on cell C_p or deleting edges in the induced subgraph K_{m_q} on cell C_q of the equitable partition π, still admits Laplacian fractional revival (resp. Laplacian PST, Laplacian PGST) between the two vertices, by Corollary 7.4.3 and Remark 7.4.4. For example, we know without calculations that the complete bipartite graph $K_{2,6}$ admits Laplacian fractional revival at time $\pi/4$ (and admits Laplacian PST at time $\pi/2$), since it can be obtained from the threshold graph $O_2 \vee K_6$ (which admits Laplacian fractional revival at time $\pi/4$ by Theorem 7.3.3, and which admits Laplacian PST at time $\pi/2$ by Theorem 7.1.4) by removing all the edges inside K_6.

Remark 7.4.6. The corresponding results about almost equitable partition of a graph can be generalized to weighted graphs, in the sense that the Laplacian matrix $L(G)$ of a weighted graph can be permuted and partitioned into a block matrix, such that all the off-diagonal blocks have constant row sums, and the corresponding row sums can be assigned to $c_{j\ell}$.

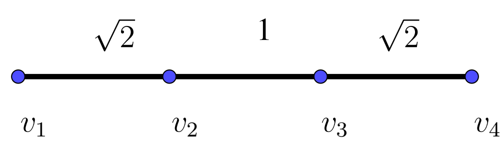


Figure 7.2: A weighted path G with adjacency fractional revival between two different pair of vertices that have one vertex in common

Example 7.4.7. Making use of the graph in Figure 7.1, Theorem 7.4.2, Definition 7.1.1, and Proposition 1.3.9, we can obtain a weighted path G as shown in Figure 7.2, which admits adjacency fractional revival between vertices v_1 and v_4 (also between v_2 and v_3) at time $t_1 = \frac{2\pi}{3}$, and adjacency fractional revival between vertices v_1 and v_3 (also between

v_2 and v_4) at time $t_2 = \pi$. Such a phenomenon cannot occur for perfect state transfer: if a graph admits perfect state transfer from vertex j to k and from j to ℓ, then $k = \ell$ (Proposition 2.6.5).

Chapter 8

Future work

In this chapter, we give a list of problems that are related to the work in this thesis.

As mentioned in Section 3.5.2, we would like to have sparse graphs that admit PST. From Corollary 3.6.2 and the fact that the n-cube admits PST at time $\pi/2$ for any positive integer n, we know that the n-cube is the sparsest graph that is diagonalizable by the standard Hadamard matrix H_n. But the standard Hadamard matrix is not the only Hadamard matrix of order 2^n for $n > 3$, for example, there are 5 non-isomorphic Hadamard matrices of order 16, and there are Hadamard matrices of some other orders apart from powers of 2, for example, there are 3 non-isomorphic Hadamard matrices of order 20. In Theorem 3.5.1 we proved that for $n \leq 4$, the n-cube is the sparsest connected Hadamard diagonalizable graphs that admit PST at time $\pi/2$. It could be interesting to determine whether the same result holds for larger n, or to check this sparsity problem among all Hadamard diagonalizable graphs that have PST (not just at time $\pi/2$).

Problem 1. *Is the n-cube the sparsest connected Hadamard diagonalizable graph that admits PST?*

In Section 3.6.2, we characterized n-cubelike graphs of degree $(n+1)$ or $(n+2)$ that admit uniform mixing at time $\pi/4$. It would be interesting to consider this property for cubelike graphs of higher degree, or alternatively, for uniform mixing at a general time.

Problem 2. *Characterize connected n-cubelike graphs of degree $d \geq n+3$ that admit uniform mixing at time $\pi/4$. Find equivalent conditions for a connected cubelike graph to admit uniform mixing.*

As mentioned in Chapter 4, it is known that the weighted path on n vertices with edge weights $w_{j,j+1} = \sqrt{j(n-j)}$ for $j = 1, \ldots, n-1$ admits adjacency PST between its end vertices, and therefore there is a weighted path that admits PST between its end vertices for any positive integer n [30]. This set of edge weights is obtained from the symmetrized quotient graph of the n-cube with respect to the distance partition. Another such set for even n is obtained by use of continued fractions and specially chosen eigenvalues [87]; using dual Hann polynomials, an edge weights set for a weighted path with loops on n vertices that admits adjacency PST between the end vertices is realized [1]. We can consider other possibilities for the edge weight set, and some necessary conditions that the edge weights need to satisfy. For instance, as shown in Example 4.4.1 and Example 4.4.2, for $n = 4$ and $n = 5$, we can produce a lot of weighted paths on n vertices that admit adjacency PST between the end vertices, by assigning proper eigenvalues to β_1 and β_2 according to Remark 4.1.9. For a general n, given a set of n distinct real numbers (eigenvalues of any weighted paths are simple) satisfying certain conditions (for example to ensure PST for a weighted path), several algorithms exist for constructing a persymmetric tridiagonal matrix (corresponding to a weighted path with or without loops) that have those numbers as eigenvalues (and hence exhibit PST) [37, 43, 87]; using these algorithms to write the persymmetric tridiagonal matrix in terms of a given set of eigenvalues satisfying Remark 4.1.9 would help us solve the problem, but there is no closed formulas to write the weights (matrix entries) in terms of eigenvalues for big n. We could also check other graphs with PST to see whether any of them admit an equitable partition π such that the symmetrized quotient graph with respect to π is a weighted path without loops.

Problem 3. *Find (or characterize) sets of edge weights for a weighted path to admit adjacency PST between the end vertices.*

Note that we already proved that no weighted path on $n \geq 3$ vertices admits Laplacian PST between its end vertices in Theorem 4.3.1. Related problems are

Problem 4. *Can a weighted path (without loops) admit Laplacian PST between its internal vertices, or between an internal vertex and an end vertex?*

Note that the answers to the above two questions are both yes under adjacency dynamics (a weighted path with adjacency PST between an internal vertex and an end vertex is constructed by Kay [60]). We have generalized Theorem 4.3.1 to certain weighted mirror symmetric trees; related future work can be to generalize it to a general weighted tree.

Problem 5. *Can a weighted tree on $n \geq 3$ vertices admit Laplacian PST?*

There is a conjecture in Chapter 4 on the edge weights of a weighted path with loops that admits adjacency PST between its end vertices at time π, that is, if all the weights of a weighted path with loops on at least 4 vertices are rational numbers, then there is no adjacency PST at time π between the end vertices of the path. We have confirmed the conjecture in cases $n = 4$, $n \equiv 3 \pmod 8$, as well as $n \equiv 5 \pmod 8$. Related future work is to prove this conjecture for other n.

Problem 6. *Prove that if all the weights of a weighted path with loops on $n \geq 4$ vertices are rational numbers, then there is no adjacency PST at time π between the end vertices of the path when n is even or $n \equiv \pm 1 \pmod 8$.*

In Chapter 5, we perform Godsil-McKay switching on the n-cube to obtain the switched n-cube, and by observation we know that $\tilde{Q}_n = Q_{n-4} \square \tilde{Q}_4$. Therefore the properties of the switched n-cube can be obtained from the $(n-4)$-cube and the switched 4-cube, or by the use of the fact that C_n and $\tilde{C}_n$ are similar through a real symmetric orthogonal matrix Q. But for a partially switched n-cube, we have much less information. We know that it shares some common eigenvalues and eigenvectors with the n-cube, but we would like to know more. Also it seems that the partially switched n-cubes have some non-integer eigenvalues, but we do not have a general proof yet.

Problem 7. *Investigate the spectral properties of partially switched n-cubes.*

We have proved that for any partially switched n-cube, at least $1/8$ of its vertices pair up to admit PST, and conjectured that this number is in fact precise.

Problem 8. *Let* $S = \{1 + 2^4 m_4 + \cdots + 2^{n-1} m_{n-1}, 16 + 2^4 m_4 + \cdots + 2^{n-1} m_{n-1} \,|\, m_k \in \{0, 1\}$ *for* $k = 4, \cdots, n-1\}$*. Prove that a vertex* j *of a partially switched* n*-cube is involved in PST if and only if* $j \in S$*.*

In Chapter 6, we have obtained bounds on the probability of state transfer for a perturbed system, where either readout time or edge weights are perturbed. We worked in the most general setting where the adjacency matrix A (or, alternatively, the Laplacian L) was arbitrary, and the perturbations themselves were arbitrary. More precise bounds can be obtained by considering more structured perturbations. Furthermore, it would be of interest to combine readout time errors with edge weight errors to create one bound encompassing both types of perturbations. Assume $\mathcal{H}$ is the Hamiltonian of a given system that admits PST at time t_0. Due to timing errors, the state is read out at time $t_0 + h$ instead. If there are also edge weight perturbations $\mathcal{H}_0$ (so the Hamiltonian is $\mathcal{H} + \mathcal{H}_0$), we could in fact see the fidelity of state transfer of the perturbed system ($\mathcal{H} + \mathcal{H}_0$) read out at the perturbed time $t_0 + h$ as the fidelity of state transfer of the perturbed system with Hamiltonian $\mathcal{H} + (\mathcal{H}_0 + \frac{h}{t_0}(\mathcal{H} + \mathcal{H}_0))$, where $\mathcal{H}_0 + \frac{h}{t_0}(\mathcal{H} + \mathcal{H}_0)$ is an edge weight perturbation of the original system, read out at (unperturbed) time t_0, thus transforming the problem to the case when only edge weight errors occur. This can be used to obtain some preliminary bounds on the fidelity when both types of errors occur.

Problem 9. *Find improved bounds on fidelity of state transfer in a perturbed system, where the unperturbed system (matrix) and the perturbation matrix are more structured, and where the unperturbed system admits PST.*

Problem 10. *For a system that admits PST, find bounds on fidelity in a perturbed system when both the readout time and edges weights are perturbed.*

Also note that our analysis for bounds on fidelity assumed perfect state transfer (PST). While there are a number of classes of graphs exhibiting PST, it is of interest to allow for pretty good state transfer (PGST) and perform a similar analysis on sensitivity of fidelity to readout time and edge weight errors; note that the numerical evidence reported in Examples 3.16 and 3.17 in [66] suggests that the fidelity may not be so well–behaved under perturbation of edge weights in the PGST setting.

Problem 11. *For a system that admits PGST, find bounds on fidelity when there is readout time error, or when there are edge weight errors, at a predetermined readout time with high fidelity.*

In Chapter 7, we considered Laplacian fractional revival of a graph, where we showed that if there is Laplacian fractional revival between two vertices j and k, then the two vertices are strongly cospectral with respect to the Laplacian matrix L. We can continue this work with the following problem.

Problem 12. *Find some other necessary conditions a graph needs to satisfy to admit Laplacian fractional revival (apart from strong cospectrality).*

For generalized fractional revival, under some special conditions, we have a result that generalizes the strong cospectrality between the two vertices with FR as mentioned in Remark 7.2.2. We have examples that do not satisfy the hypothesis that 1 is a simple eigenvalue of $U_1 = U(t)_{[S,S]}$. A related future problem can be the following.

Problem 13. *Assume a graph G admits generalized Laplacian fractional revival at time t between the set of vertices $S \subset V(G)$ with $2 < |S| < |V(G)|$. Investigate what types of graphs satisfy the condition that 1 is a simple eigenvalue of $U(t)_{[S,S]}$. Check the Laplacian fractional revival property of some other family of graphs.*

We can start with the class of graphs with only integer Laplacian eigenvalues, of which threshold graphs are members.

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