Quantum pure state transfer

by

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Abstract

Quantum spin systems carry information in the form of quantum states, and the propagation of these quantum states is described by a quantum walk. In order to construct an operational quantum computer, the task of reliably transmitting quantum states from one part of a quantum computer to another must be accomplished. Quantum walks are known to be powerful tools in achieving this task.

Pure states are quantum states represented by unit complex vectors. In this thesis, we use algebraic and combinatorial techniques to develop the theory of perfect state transfer on pure states in quantum walks, with emphasis on the adjacency and Laplacian matrices as Hamiltonians of a graph representing a spin network.

We prove basic results about eigenvalue supports, periodicity, and strong cospectrality on pure states. We investigate a special type of strong cospectrality called m-strong cospectrality, and show that m-strongly cospectral pure states admit desirable quantum state transfer properties. Several characterisations of perfect state transfer are also given, one for general pure states, one for m-strongly pure states, and another one for real pure states. These characterisations give rise to algebraic and analytic properties of pure states admitting perfect state transfer. Moreover, we determine all complete graphs, complete bipartite graphs, cycles, and paths that admit perfect state transfer between m-strongly pure states. Constructions of infinite families of graphs admitting perfect state transfer are also given.

We also characterise perfect state transfer between vertex states in joins and blow-up graphs. We determine when the join operation preserves or induces perfect state transfer in the resulting graph. We also use blow-up graphs to construct new families of regular graphs with perfect state transfer. We use these two graph operations to demonstrate that graphs with perfect state transfer can be constructed from graphs that do not exhibit such a property.

Finally, we investigate perfect state transfer on s-pair states – pure states that represent entanglement between two vertices. We establish combinatorial and spectral properties of s-pair states with perfect state transfer, and characterise its existence in complete graphs, complete bipartite graphs, paths and distance-regular graphs. Further, we construct infinite families of graphs with s-pair state transfer.

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To Mama Nene.
To Papa Junjun.
To Tatay Metes.

Contents

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$\mathbb{R}$	the set of real numbers
$\mathbb{C}$	the set of complex numbers
$\mathbb{Q}$	the set of rational numbers
$\mathbb{Z}$	the set of integers
$\mathbb{Z}_n$	the set of integers mod n
X	a simple undirected weighted graph
$V(X)$	the vertex set of X
$E(X)$	the edge set of X
$N_X(u)$	the set of neighbours of vertex u in X
$X \backslash u$	the resulting graph after deleting vertex u from X
$X_1 \cup X_2$	the union of two graphs X_1 and X_2
$X_1 \vee X_2$	the join of two graphs X_1 and X_2
$X_1 \square X_2$	the Cartesian product of two graphs X_1 and X_2
$X_1 \times X_2$	the direct product of two graphs X_1 and X_2
$X^{\square n}$	the Cartesian product of n copies of X
$\overset{n}{\uplus} X$	the blow-up of n copies of X
C_n	the cycle on n vertices
K_n	the complete graph on n vertices
$K_{a,b}$	the complete bipartite graph with partite sets of sizes a and b
O_n	the empty graph on n vertices
P_n	the path on n vertices
Q_n	the hypercube of dimension n, also known as the n-cube
$CP(n)$	the cocktail party graph on $2n$ vertices
$D(X)$	the degree matrix of a graph X
$A(X)$	the adjacency matrix of a graph X
$L(X)$	the Laplacian matrix of a graph X

$\alpha D(X) + A(X)$	a generalised adjacency matrix of a graph X, where $\alpha \in \mathbb{R}$
$M(X)$	a real symmetric matrix associated with a graph X
$U(t)$	the transition matrix of a graph X with respect to $M(X)$
E_λ	the orthogonal projection matrix associated with $\lambda \in \operatorname{spec}(M)$
$\operatorname{spec}(M(X))$	the set of distinct eigenvalues of $M(X)$
$\Phi_{\mathbf{x}}(M(X))$	the eigenvalue support of a complex vector $\mathbf{x}$ relative to $M(X)$
$\Phi^{\pm}_{\mathbf{x},\mathbf{y}}(M(X))$	the set of all eigenvalues $\lambda \in \Phi_{\mathbf{x}}(M(X))$ such that $E_\lambda \mathbf{x} = \pm E_\lambda \mathbf{y}$
$\phi(M, t)$	the characteristic polynomial of a matrix M in the variable t
$\lVert \mathbf{x} \rVert$	the Euclidean norm of a vector $\mathbf{x} \in \mathbb{C}^n$
$A \circ B$	the Schur (Hadamard) product of matrices A and B
$A \otimes B$	the tensor product of matrices A and B
$A^{\otimes n}$	the tensor power of the matrix A with itself n times
A^T	the transpose of a matrix A
A^*	the conjugate transpose of a matrix A
$\mathbf{x}^T$	the transpose of a vector $\mathbf{x}$
$\mathbf{x}^*$	the conjugate transpose of a vector $\mathbf{x}$
$J_{m,n}$	the all-ones $m \times n$ matrix
J_n	the all-ones $n \times n$ matrix
I_n	the identity $n \times n$ matrix
$\mathbf{1}_n$	the all-ones vector in $\mathbb{C}^n$
$\mathbf{0}_n$	the all-zeros vector in $\mathbb{C}^n$
$\mathbf{e}_1, \ldots, \mathbf{e}_n$	the standard basis vectors for $\mathbb{C}^n$
$\lvert a \rvert$	the modulus of a complex number a
$\nu_p(a)$	the p-adic valuation of an integer a
$\operatorname{lcm}(a, b)$	the least common multiple of integers a and b
$\gcd(a, b)$	the greatest common divisor of integers a and b
$\rho_{\mathbf{x}}$	the minimum period of a complex vector $\mathbf{x}$
$\mathbf{e}_S$	the characteristic vector of a nonempty subset S of $V(X)$
$\mathbf{e}_u$	the characteristic vector of vertex u
$\mathbf{e}_u$	the vertex state associated with vertex u in X
$\mathbf{e}_u + \mathbf{e}_v$	the plus state associated with two vertices u, v in X
$\mathbf{e}_u - \mathbf{e}_v$	the pair state associated with two vertices u, v in X
$\mathbf{e}_u + s\mathbf{e}_v$	an s-pair state associated with two vertices u, v in X

1

Introduction

In quantum information theory, *quantum states* encode quantum information. However, unlike classical states which obey classical physics, quantum states exhibit two intriguing properties derived from quantum mechanics. The first is *quantum superposition*, which is the ability of a quantum system to exist in multiple states at once until observed. Schrödinger's cat is a classic example of a thought experiment that demonstrates this property [82]. The second is *quantum entanglement*, which allows quantum states to interact regardless of distance. Quantum computers exploit these two properties, hopefully allowing them to process huge amounts of data. As a result, quantum computers represent a profound leap in computational capabilities compared to their classical counterparts. Although the construction of practical quantum computers is still in its early stages, quantum computers bring the promise of revolutionising scientific computing. For this reason, quantum computing has attracted a great deal of attention in the last few decades.

In order to build an operational quantum computer, the task of reliably transmitting quantum states from one part of a quantum computer to another must be achieved. The carrier of these quantum states from one register to another within a quantum computer is called a *quantum spin network*, which can be modeled by an undirected weighted graph whose vertices and edges represent qubits and their interactions in the spin network, respectively. The propagation of quantum states within a spin network is described by a *quantum walk*, which is a probabilistic process determined by a unitary matrix derived from the Hamiltonian of the spin network.

To transmit a quantum state within a quantum computer, a quantum state is first initialised. In this case, one ideally has full knowledge of the initial state of the spin network, and so one may consider such a state as a *pure state* [72], which is a quantum state represented by a unit complex vector. Once the spin network is isolated from the external environment, the initial state dynamically evolves over time, in the hope of getting transmitted to a target quantum state with high probability. *Perfect state transfer* is achieved if the initial state is transmitted to the target quantum state with probability one at a later time (up to a phase factor).

Due to its practical applications, the study of perfect state transfer (and more generally, quantum walks) has become an indispensable area within the theory of quantum computation since its introduction two decades ago. In this thesis, we aim to contribute to the existing body of work on perfect state transfer by thoroughly examining its occurrence on pure states. Our work herein offers one of the most general treatment of perfect state transfer thus far, and provides a framework that unifies numerous results on perfect state transfer in the literature. In particular, we use algebraic and combinatorial approaches to address our main goals in this thesis:

1. Establish a relationship between the spectral properties of a Hermitian matrix that respects the adjacencies of a given graph and the occurrence of perfect state transfer on pure states.

2. Construct graphs that admit perfect state transfer on pure states.

3. Understand the influence of the underlying structure of the graph on the occurrence of perfect state transfer on pure states.

4. Determine the inherent properties of pure states that affect their ability to exhibit perfect state transfer.

5. Identify the differences in behaviour between quantum walks defined using different matrices associated with the same underlying graph.

1.1 Motivation

A quantum spin network consisting of n *qubits* (also known as *spins*) can be viewed as an undirected weighted graph X on n vertices whose vertex set $V(X)$ and edge set $E(X)$ consist of the qubits and their interactions in the network, respectively. The weight of an edge between two qubits in X can be physically interpreted as the *coupling strength* between them, while the weight of a loop on a qubit in X can be viewed as a *potential* on the qubit (also called *energy shift*), which represents the strength of the magnetic field on the qubit [13, 19].

A qubit is a quantum analogue of a classical bit. Mathematically speaking, a qubit in a spin network is associated with a two-dimensional complex vector space

$\mathbb{C}^2$, and the state of a qubit can be expressed as a unit vector in $\mathbb{C}^2$. The spin network is initialised by assigning quantum states to the qubits in the network. The state of the whole quantum spin network is obtained taking the tensor product of the states of the n qubits, and such a quantum state is represented as a unit vector in $\mathbb{C}^{2^n}$. Without the presence of external control, we let the resulting *quantum spin system* dynamically evolve over time. In this case, the propagation of the system depends uniquely on the initial state, the structure of the spin network, and the choice of dynamics of the system (which, as we will see later on, corresponds to a real symmetric matrix associated with a graph representing the spin network).

The *Hamiltonian* $\mathcal{H}$ of a quantum spin network is a time-independent Hermitian matrix that depends on the dynamics governing the evolution of the network. If $\varphi(t)$ denotes the state of the quantum spin system at time t with Hamiltonian $\mathcal{H}$, then its evolution adheres to *Schrödinger's equation* [72, Equation II.16, pp. 64]:

$$\mathrm{i}\hbar\frac{d}{dt}\varphi(t) = \mathcal{H}\varphi(t),$$

where $\hbar = \frac{h}{2\pi}$ and h is Planck's constant. Consequently, the state of the spin system at any time $t \in \mathbb{R}$ is given by

$$\varphi(t) = U(t)\varphi(0), \tag{1.1.1}$$

where $\varphi(0)$ is the initial state of the system, and

$$U(t) = e^{-i\mathcal{H}t/\hbar}, \quad t \in \mathbb{R}$$

is a unitary matrix called the *transition matrix* of the quantum walk relative to $\mathcal{H}$. The matrix $U(t)$ determines a *(continuous) quantum walk* on X, which is a probabilistic process that describes the propagation of quantum states in the spin network. Moreover, if we let $\tau = -t/\hbar$, then we may simplify $U(t)$ above as

$$U(\tau) = e^{i\mathcal{H}\tau} \quad \tau \in \mathbb{R}. \tag{1.1.2}$$

In this thesis, we restrict our attention to the single excitation subspace of $\mathbb{C}^{2^n}$, which is the subspace spanned by the vectors $\mathbf{e}_1, \dots, \mathbf{e}_n$, where $\mathbf{e}_u$ is the standard basis vector associated with qubit u. In this case, $\mathbf{e}_u$ indicates the presence of the excitation on qubit u and absence on all the others. This additional assumption reduces the size of our Hamiltonian $\mathcal{H}$ to $n \times n$ in lieu of $2^n \times 2^n$ [31], and yields the initial state

$$\varphi(0) \in \mathbb{C}^n. \tag{1.1.3}$$

Once the initialisation of the spin network is complete, then we have full knowledge of the quantum state of the spin system, and so we may assume that $\varphi(0)$ in this case is a pure state. Equations (1.1.2) and (1.1.3) then allow us to define perfect state transfer on pure states in a matrix-theoretic fashion in Chapter 4.

We now demonstrate that under certain dynamics, the Hamiltonian $\mathcal{H}$ can be taken to be the adjacency or (combinatorial) Laplacian matrix of X. Consider the *Pauli matrices*

$$\sigma^x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma^y = \begin{bmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{bmatrix} \quad \text{and} \quad \sigma^z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$

For a given qubit u in X and a Pauli matrix $w \in \{x, y, z\}$, let σ_u^w be the $2n \times 2n$ matrix obtained by taking the tensor product of $u-1$ copies of I_2, followed by a copy of σ^w, and then followed by $n-u$ copies I_2, where I_2 is the 2×2 identity matrix. The matrix σ_u^w represents the action of a Pauli matrix on qubit u in the direction w. Via nearest-neighbour interaction, a common form of the Hamiltonian is given by

$$\mathcal{H} = \frac{1}{2} \sum_{\{u,v\} \in E(X)} (J_x \sigma_u^x \sigma_v^x + J_y \sigma_u^y \sigma_v^y + J_z \sigma_u^z \sigma_v^z), \tag{1.1.4}$$

where $J_w \in \mathbb{R}$ is the strength of the coupling in the direction w of spin interaction with $w \in \{x, y, z\}$ [13].

Typically, there are two types of dynamics, one determined by the `XY` model (also called `XX`), and the other by the `XYZ` model (also called *Heisenberg* or `XXX`). For the `XY` model, the Hamiltonian is taken to be the adjacency matrix of X. To demonstrate this fact, suppose the dynamics of our spin system is determined by the `XY` model. This means that interaction of spins along the z direction absent, and so we may set $J_x = J_y = 1$ and $J_z = 0$ in (1.1.4) to obtain

$$\mathcal{H} = \frac{1}{2} \sum_{\{u,v\} \in E(X)} (\sigma_u^x \sigma_v^x + \sigma_u^y \sigma_v^y). \tag{1.1.5}$$

Using the properties of Pauli matrices, an uninteresting computation reveals that $\mathbf{e}_j^T \sigma_u^x \sigma_v^x \mathbf{e}_k = \mathbf{e}_j^T \sigma_u^y \sigma_v^y \mathbf{e}_k = \delta_{j,u}\delta_{k,v}$ where $\delta_{j,k} = 1$ if $j = k$ and $\delta_{j,k} = 0$ otherwise.

Thus, if $j, k \in V(X)$ are spins in our network, then (1.1.5) gives us

$$\mathbf{e}_j^T \mathcal{H} \mathbf{e}_k = \sum_{\{u,v\} \in E(X)} \delta_{j,u}\delta_{k,v} = \begin{cases} 1, & \text{if } \{j,k\} \in E(X) \\ 0, & \text{otherwise} \end{cases}.$$

Consequently, for the `XY` model, the action of $\mathcal{H}$ on the single excitation subspace of $\mathbb{C}^{2^n}$ is equivalent to the action of the adjacency matrix of X on $\mathbb{C}^n$. In [14], it was shown that for the `XYZ` model, the action of $\mathcal{H}$ on the single excitation subspace of $\mathbb{C}^{2^n}$ is equivalent to the action of the Laplacian matrix of X on $\mathbb{C}^n$.

While the adjacency and Laplacian matrix are the common choices of Hamiltonian in the literature, we note in general that $\mathcal{H}$ may be taken to be any Hermitian matrix having the property that the entry of $\mathcal{H}$ indexed by vertices u and v of X is zero if and only if there is no edge between u and v [23]. That is, regardless of edge weights, $\mathcal{H}$ combinatorially respects the adjacencies of the vertices in X. In particular, for our work, the theory we develop for perfect state transfer on pure states apply to any real symmetric Hamiltonian, although we often specify that the Hamiltonian taken is the adjacency or the Laplacian matrix of the graph.

1.2 Brief literature review

This thesis is primarily concerned with continuous quantum walks, which are distinct from discrete quantum walks. For more information on discrete quantum walks, we refer the reader to [57, 84, 86].

The concept of a continuous quantum walk was first introduced by Farhi and Gutmann [44] in 1998 to move through decision trees. They showed that the complexity of quantum algorithms on decision trees via a quantum walk is, in some cases, faster than the complexity of classical algorithms via a continuous random walk. However, it was not until 2003 when Bose proposed the use of unweighted paths (also known as uniformly coupled spin chains in physics) to transmit quantum states (in the form of vertex states) for short distance communication [13]. These unweighted paths represent the quantum wires between distinct quantum registers, which are necessary in building a powerful quantum computer. For economic purposes, it is desirable to minimise the number of interactions between the qubits in these quantum wires. Hence, the use of paths in this endeavour is natural, as they have the largest diameter amongst all graphs on a fixed number of vertices.

Motivated by accurate transmission of quantum information, Christandl et al.

introduced the concept of perfect state transfer between vertex states in a graph in 2005 [31], and showed that unweighted paths on n vertices only admit perfect state transfer between end vertices for $n = 2$ or $n = 3$ relative to the adjacency matrix, and $n = 2$ relative to the Laplacian matrix [30]. This prompted researchers to search for new graphs admitting perfect state transfer between vertex states. Some infinite families with this desirable property include cubelike graphs [29], integral circulant graphs [10], distance-regular graphs [38], Hadamard diagonalisable graphs [60], and quotient graphs [6, 45]. Perfect state transfer between vertex states has also been investigated in certain joins of graphs [2, 3], signed graphs [18], products and covers of graphs [35] and non-complete extended p-sums (NEPS) of some graphs [70, 81].

Trees are also of great interest, as they are the sparsest connected graphs amongst all graphs on a fixed number of vertices. However, Coutinho and Liu showed in 2015 that unweighted trees on n vertices admit perfect state transfer between vertex states relative to the Laplacian matrix if and only if $n = 2$ [41], thereby extending the result of Christandl et al. from paths to trees. More recently, Coutinho, Juliano and Spier showed that the result of Christandl et al. relative to the adjacency matrix also holds for unweighted trees in general [40]. To make matters worse, Godsil proved in 2012 that for every positive integer k, there are only finitely many unweighted graphs with maximum degree k admitting perfect state transfer between vertex states [50]. Consequently, amongst unweighted graphs, the existence of perfect state transfer between vertex states is rare, and if it does happen, then we can say for certain that the graph is not a tree. This rarity encouraged researchers to continue the search for unweighted graphs admitting this property [5, 71]. For surveys about perfect state transfer between vertex states, we refer the reader to [50, 61, 63]. For a more self-contained treatment of this topic, please see [32, 38, 73, 87].

To get around the rarity of perfect state transfer between vertex states in unweighted graphs, some authors explored whether weighting edges as well as adding weighted loops to some vertices of the graph can produce perfect state transfer between vertex states [2, 3, 19, 31, 62, 65]. Several authors also investigated the potency of certain graph operations in preserving or inducing perfect state transfer between vertex states in the resulting graph, such as the join operation [66] and the blow-up operation [12]. Moreover, some researchers considered generalisations of perfect state transfer. In 2012, Godsil [50], and Vinet and Zhedanov [85] independently introduced the notion of pretty good state transfer between vertex states, which is a less stringent version of perfect state transfer. It turns out that an infinite family of unweighted paths exhibit pretty good state transfer as demonstrated by Godsil et al. [54] and van Bommel [83] relative to the adjacency matrix, and Banchi et al. relative to the Laplacian matrix [7]. Another generalisation of perfect state transfer between vertex states is fractional revival. Earlier publications on fractional revival in the context of quantum state transfer date back to 2016 [47], and possibly earlier. Later on, the role of the underlying graph structure was investigated in relation to the occurrence of fractional revival [21, 22, 23, 68, 75].

A more recent generalisation of perfect state transfer is called *s-pair state transfer*, whereby one is interested in whether an entangled (ordered) pair of vertices admits perfect state transfer with another entangled pair of vertices. An entangled pair of vertices (u, v) is represented by an s-pair state $\mathbf{e}_u + s\mathbf{e}_v$, where $s \in \mathbb{C}\backslash\{0\}$ determines the level of entanglement between vertices u and v. Thus, s-pair state transfer is perfect state transfer between entangled states. Chen first studied s-pair state transfer when $s = \pm 1$ and the pairs of vertices form edges in the graph [27]. After noticing that s-pair state transfer happens between pairs of vertices that do not form edges, Chen and Godsil extended Chen's work to include any pair of vertices in the graph [28]. Other work related to s-pair state transfer where $s = \pm 1$ can be found in [11, 80]. Later on, a more general framework in studying s-pair state transfer for arbitrary $s \in \mathbb{R}\backslash\{0\}$ was provided by Chan et al. [64].

The most up-to-date work on perfect state transfer is due to Godsil, Kirkland and Monterde, where they investigated perfect state transfer between real pure states [53], which includes the class of vertex states and s-pair states with $s \in \mathbb{R}\backslash\{0\}$. They provided a characterisation of perfect state transfer between real pure states that generalises Coutinho's result for vertex states [32]. It turns out that periodicity of a real pure state is a sufficient condition for perfect state transfer, unlike the case of a vertex state where strong cospectrality and number-theoretic conditions on eigenvalues in the support are also required. They also showed that real pure states with eigenvalue supports of size two admit perfect state transfer. This is in stark contrast to perfect state transfer between vertex states where eigenvalue supports are required to have sizes at least three whenever the graph has at least three vertices.

1.3 Summary and structure of this thesis

The emergence of new studies on perfect state transfer between s-pair states and real pure states motivates an investigation of perfect state transfer involving pure states in general. In this thesis, our main goal is to utilise algebraic and combinatorial approaches to develop the theory of perfect state transfer on pure states in continuous quantum walks. We bring forth several characterisations and various constructions of graphs admitting perfect state transfer, and analyze the algebraic, analytic and combinatorial properties of pure states that exhibit perfect state transfer. Our work represents a new line of inquiry and a unified framework in studying perfect state transfer in quantum spin networks. We organise this thesis as follows, giving emphasis to the new results in each chapter from Chapter 4 to Chapter 9.

Chapter 2 gives a compilation of definitions, basic notation, and useful facts from graph theory, matrix theory, algebra, and number theory, which provides all the necessary background for the reader.

Our goal in Chapter 3 is to provide an overview of quantum state transfer involving pure states. We establish basic results about concepts that are useful throughout this work, such as eigenvalue supports, periodicity, and strong cospectrality. We explore a special type of strong cospectrality called m-strong cospectrality. We also review quantum walks built using graph operations.

In Chapter 4, we develop the theory of perfect state transfer on pure states. We provide spectral characterisations of perfect state transfer, which yield three fundamental results: (i) every periodic pure state $\mathbf{x}$ admits perfect state transfer with another pure state $\mathbf{y}$ such that $\mathbf{x}$ and $\mathbf{y}$ are m-strongly cospectral, (ii) every connected graph admits perfect state transfer between real pure states, and (iii) for any pair of pure states $\mathbf{x}$ and $\mathbf{y}$ and for any time $\tau > 0$, there exists a Hermitian matrix M such that $\mathbf{x}$ and $\mathbf{y}$ admits perfect state transfer relative to the quantum walk on M at time τ. We establish algebraic and analytic properties of pure states admitting perfect state transfer. We also investigate whether the desirable properties of perfect state transfer between vertex states, namely monogamy, symmetry and minimum PST time, extend to m-strongly cospectral pure states. We also present several constructions of graphs admitting perfect state transfer on pure states.

Chapter 5 is dedicated to providing a number-theoretic characterisation of perfect state transfer between m-strongly cospectral pure states. We determine all complete graphs, complete bipartite graphs, cycles and paths that admit perfect state transfer between m-strongly pure states. For fixed $m, n \geq 2$, we also determine the pure states and the families of unweighted graphs that achieve the least minimum PST time amongst all unweighted graphs on n vertices and all m-strongly cospectral pure states in $\mathbb{C}^n$ relative to the adjacency and the Laplacian matrix.

Real pure states are discussed in Chapter 6. We characterise weak and strong cospectrality on real pure states, and show that periodicity of nonnegative rational states is a rare phenomenon. We provide a characterisation for perfect state transfer between real pure states and show that such a characterisation coincides with that of perfect state transfer on m-strongly cospectral pure states with $m = 2$. We show that strong cospectrality between real pure states is a special case of m-strong cospectrality, and so we recover the properties of real pure states admitting perfect state transfer from that of m-strongly cospectral pure states. We also survey results on unweighted graphs that admit perfect state transfer between real pure states.

In Chapters 7 and 8, we contribute to the existing body of work on perfect state transfer between vertex states by characterising strong cospectrality and perfect state transfer in join graphs and blow-up graphs, respectively. In particular, in Chapter 7, we determine under which conditions is perfect state transfer between vertex states preserved or induced in a join graph. We also show that the quantum walks determined by a graph and its join become equivalent when restricted to the vertices of the graph, as the graph becomes larger. Meanwhile, in Chapter 8, we demonstrate how the blow-up operation can be used to construct larger graphs with perfect state transfer between vertex states. Like join graphs, blow-up graphs in some cases can be used to generate infinite families of graphs with perfect state transfer from graphs that do not admit such a property. We also prove that if the graph has a number of vertices that is a multiple of four, then under certain conditions, the addition of an appropriate matching in the blow-up graph results in perfect state transfer between the vertices corresponding to the newly added edges.

Chapter 9 is devoted to the theory of s-pair state transfer, where $s \in \mathbb{C}\backslash\{0\}$. We establish algebraic and combinatorial properties of strongly cospectral s-pair states. We characterise s-pair state transfer in complete graphs, complete bipartite graphs, paths, cycles and antipodal distance-regular graphs with vertex perfect state transfer. We also provide constructions of s-pair states that admit perfect state transfer. This leads to new interesting families of graphs exhibiting s-pair state transfer.

Finally, to inspire further work on this topic, we present several open questions in Chapter 10.

2

Background

In this chapter, we provide an overview of the concepts relevant to this work. We start by introducing standard definitions and notation from graph and matrix theory.

2.1 Basic definitions and notation

A *graph* X is a pair $(V(X), E(X))$, where $V(X) \neq \varnothing$ is the *vertex set* of X and $E(X)$ is the *edge set* of X . The elements of $V(X)$ are called *vertices* while those in $E(X)$ are called *edges*, which are ordered pairs of vertices in $V(X)$. If $(u, v) \in E(X)$, then we say that vertex u is *adjacent* to vertex v, and the edge (u, v) is *incident* to vertex v. If the edges in X are unordered pairs of vertices, then we say that X is an *undirected graph.* In an undirected graph X, the adjacency relation between vertices is symmetric. In this case, we write the edge between u and v as $\{u, v\}$, and we say that $\{u, v\}$ is incident to both u and v. We also say that vertices u and v are neighbours if u and v are adjacent, and we denote the set of neighbours of v in X by $N_X(v)$. An edge of the form $\{v, v\}$ is called a *loop* on v, and in this case, we say that v is adjacent to itself. A graph X is *simple* if its edge set is not a multi-set and it does not contain loops. A *weighted graph* is a graph whose edges are assigned a positive real number, called the *weight* of the edge. In particular, if the weights are all one, then we say that the weighted graph (resp., weighted directed graph) is *unweighted.* That is, an unweighted graph is a special case of a weighted graph. Unless otherwise stated, we assume all graphs to be undirected, simple and weighted, where the edge weights are all positive. For the basics of graph theory, see [26].

The *degree* of a vertex v in a graph, denoted $\deg(v)$, is the sum of the weights of the edges incident to v. In an unweighted graph, the degree of a vertex v is the number of edges incident to v. A path of length ℓ from vertex u to vertex v in a graph is a sequence of $\ell+1$ distinct vertices starting with u and ending with v such that any two consecutive vertices are adjacent. We say that a graph X is *connected* if for every pair of vertices in X, there is a path that joins them. Otherwise, X is *disconnected.* We say that vertex u is *isolated* in X if $\deg u = 0$, or equivalently, there are no edges incident to vertex u. Note that a graph on at least two vertices with an isolated vertex is disconnected. A *matching* on a graph X is a set of edges that do not have common vertices. A *perfect matching* is a matching such that every vertex of the graph is incident to an edge of the matching.

Let X be a weighted graph. If X has no edges, then X is the *empty graph* on n vertices denoted by O_n. If any two vertices of X are adjacent, then X is a *complete graph* on $n \geq 3$ vertices. The unweighted complete graph on $n \geq 2$ vertices is denoted by K_n. We say that X is *weighted k-regular* if every vertex of X has degree k. A *path* on $n \geq 3$ vertices is a graph with vertex set $\{1, 2, \dots, n\}$ and edge set $\{\{j, j+1\} : j = 1, \dots, n-1\}$. We denote the unweighted path on n vertices by P_n. A *cycle* on $n \geq 3$ vertices is a graph with vertex set $\mathbb{Z}_n$ and vertices j, k of C_n are adjacent whenever $|k-j| \equiv 1 \pmod{n}$. Note that C_n is obtained when the two end vertices of P_n are joined. A graph X is *bipartite* if $V(X)$ can partitioned into subsets V_1 and V_2, called *partite sets*, such that each edge of X has one end vertex in V_1, and the other end vertex in V_2. If all edges in a bipartite graph are present, then we say that X is a *complete bipartite graph* on $a = |V_1|$ and $b = |V_2|$ vertices. We denote the unweighted complete bipartite graph by $K_{a,b}$.

A graph Y is a *subgraph* of a graph X if $V(Y) \subseteq V(X)$ and $E(Y) \subseteq E(X)$. A subgraph Y of X is *induced* if two vertices in Y are adjacent if and only if they are adjacent in X. A connected subgraph of X that is maximal is called a *component* of X. A *tree* is a connected graph that does not contain any cycles as subgraphs. A *spanning tree* of a graph X is a subgraph of X that is a tree that contains all vertices of X. Note that a graph has a spanning tree if and only if it is connected. For a vertex u in a graph X, we use $X \backslash u$ to denote the induced subgraph of $V(X) \backslash \{u\}$ which is called a *vertex-deleted* graph. The *union* $X_1 \cup X_2$ of graphs X_1 and X_2 with disjoint vertex sets is the graph such that $V(X_1 \cup X_2) = V(X_1) \cup V(X_2)$ and $E(X_1 \cup X_2) = E(X_1) \cup E(X_2)$.

Next, we consider basic definitions and notation from matrix theory. We refer the reader to [59] for standard concepts in matrix theory.

We use $\mathbf{1}_n$ to denote the all ones column vector of length n, we use I_n to denote the identity $n \times n$ matrix, we use $J_{m,n}$ to denote the all ones $m \times n$ matrix, and we use $\mathbf{0}_n$ to denote the all zeros column vector of length n. If $m = n$, then we denote

$J_{m,n}$ by J_n. We omit the subscripts of $\mathbf{1}_n$, I_n, $J_{m,n}$, $\mathbf{0}_n$, and J_n if their sizes are clear from the context. We write the *standard basis vectors* in $\mathbb{C}^n$ as $\mathbf{e}_1, \ldots, \mathbf{e}_n$. If X is a graph with $V(X) = \{1, \ldots, n\}$, then we denote the *characteristic vector* of vertex $u \in V(X)$ using the standard basis vector $\mathbf{e}_u$. The *characteristic vector* of a subset S of $V(X)$, denoted $\mathbf{e}_S$, is defined as $\mathbf{e}_S = \sum\limits_{u \in S} \mathbf{e}_u$, which is the vector with a 1 at an entry indexed by a vertex in S and 0's elsewhere. If $S = \{u\}$, then the characteristic vector of S is simply $\mathbf{e}_u$, the characteristic vector of vertex u.

Let A be an $m \times n$ matrix. We say that A is a *complex* (*real*, *nonnegative*, respectively) matrix if A is entry-wise complex (real, nonnegative, respectively). We denote the entry of A in the j-th row and ℓ-th column by $(A)_{j,\ell}$ for all $1 \leq j \leq m$ and $1 \leq \ell \leq n$. The entries of the form $(A)_{\ell,\ell}$ are called the diagonal entries of A. We denote the *transpose* of A by A^T. If A is a complex matrix, then we denoted by $\overline{A}$ the matrix derived from A by taking the conjugates of all its entries. We then use A^* to represent the conjugate transpose $(\overline{A})^T$. Note that if A is a real matrix, then $A^* = A^T$. If B is an $p \times q$ matrix, then the *tensor product* of A and B, denoted $A \otimes B$, is the $mp \times nq$ matrix which can be partitioned into mn blocks with the same size as B, where the (j, ℓ) block is $a_{j,\ell}B$. If B is an $n \times n$ matrix, then the *Schur product* $A \circ B$ is the matrix whose entries are the entrywise product of A and B. That is, $(A \circ B)_{j,\ell} = (A)_{j,\ell}(B)_{j,\ell}$.

Let A be an $n \times n$ matrix. We say that A is *Hermitian* if $A = A^*$, *skew-Hermitian* if $A = -A^*$, *symmetric* if $A = A^T$, and *idempotent* if $A^2 = A$. If A is real symmetric, then A is Hermitian. If A is Hermitian, then iA is skew-Hermitian. We say that A is *diagonal* if all non-diagonal entries of A are zero, in which case we can write $A = \text{diag}(a_1, a_2, \ldots, a_n)$, where a_j is the diagonal entry on the j-th row and column of A. We say that A is a *doubly stochastic matrix* if it is a nonnegative matrix whose sum of all entries in each row and each column is one. We say that A is *hollow* if each diagonal entry of A is equal to zero.

A *permutation matrix* P is a square matrix whose entries are either 0 or 1, and the entry 1 appears exactly once in each row and column of P. A permutation matrix P is known to satisfy $P^TP = PP^T = I$. A complex square matrix U is called *unitary* if $UU^* = U^*U = I$. If we also assume that U is real, then U is said to be an *real orthogonal matrix.* Consequently, any permutation matrix is a real orthogonal matrix. A square matrix A is *reducible* if it is permutation similar to a matrix in block-diagonal form. A square matrix that is not reducible is said to be *irreducible.*

We denote complex vectors using lowercase letters in boldface, like $\mathbf{x}$ and $\mathbf{y}$. If $\mathbf{x} \in \mathbb{C}^n$, then the *Euclidean norm* of $\mathbf{x}$ is given by $\|\mathbf{x}\| = \sqrt{\mathbf{x}^*\mathbf{x}}$. The Euclidean norm is *unitarily invariant*, that is, $\|U\mathbf{x}\| = \|\mathbf{x}\|$ for any unitary matrix U.

The *characteristic polynomial* of a square matrix A, denoted by $\phi(A,t)$, is the polynomial $\phi(A,t) = \det(tI - A)$. A root λ of $\phi(A,t)$ is called an *eigenvalue* of A. We denote the set of all distinct eigenvalues of A by $\operatorname{spec}(A)$. The *algebraic multiplicity* of an eigenvalue λ of A refers to the multiplicity λ as a root of $\phi(A,t)$. We say that λ is a *simple* eigenvalue of A if its algebraic multiplicity is one. For an eigenvalue λ of A, a non-zero vector $\mathbf{w}$ such that $A\mathbf{w} = \lambda\mathbf{w}$ is called an *eigenvector* associated with λ. The *eigenspace* of λ is the vector space of all eigenvectors associated with λ. The trace of A, which is the sum of all diagonal entries of A, is equal to the sum of all eigenvalues of A counting multiplicity, while the determinant of A is equal to the product of all eigenvalues of A counting multiplicity.

It is widely known that the eigenvalues of every Hermitian matrix are all real. A Hermitian matrix whose eigenvalues are all positive (resp., nonnegative) is called *positive definite* (resp., *positive semidefinite*). In fact, a matrix A is positive semidefinite (resp., positive definite) if we can write $A = BB^*$ for some rectangular (resp., invertible) matrix B. It is also well-known via the *Perron-Frobenius Theorem* that if A is an irreducible nonnegative matrix, then the largest eigenvalue of A, called the *Perron eigenvalue*, is positive and simple, and has an associated eigenvector that has all entries positive, called a *Perron eigenvector* [59, Chapter 8].

2.2 Graphs and matrices

We now review some concepts in graphs and matrices that are crucial in this work. We refer the reader to [8, 55] for further reading on this topic.

Let X be an undirected weighted graph on n vertices labelled from 1 to n. By a *real symmetric matrix that (combinatorially) respects the adjacencies* in X, we mean a real symmetric matrix M such that $M_{u,v} \neq 0$ whenever $\{u,v\}$ is an edge in X and $u \neq v$. In particular, we do not place any restrictions on the diagonal entries of M. That is, M may or may not be hollow.

The *adjacency matrix* $A(X)$ of X is the $n \times n$ matrix given by

$$A(X)_{u,v} = \begin{cases} \omega_{\{u,v\}}, & \text{if } u \text{ and } v \text{ are adjacent} \\ 0, & \text{otherwise,} \end{cases}$$

where $\omega_{\{u,v\}}$ is the weight of the edge $\{u,v\}$. If X is unweighted, then $\omega_{\{u,v\}} = 1$ whenever u and v are adjacent. Since X is undirected, $A(X)$ is a symmetric matrix.

The *degree matrix* $D(X)$ of X is the diagonal matrix whose j-th diagonal entry is the degree of vertex j. Note that $A(X)$ and $D(X)$ both only have nonnegative entries.

An *incidence matrix* B of X is a matrix whose rows and columns are indexed by the vertices and edges of X respectively, and $B_{u,e} = \omega_e$ if vertex u is incident to edge e with weight ω_e and $B_{u,e} = 0$ otherwise. Note that each column of B has exactly two nonzero entries, which are both equal to the weight of the edge indexed by that column. An *oriented incidence matrix* C of X is obtained from the incidence matrix of X by replacing exactly one of the two nonzero entries in each column of B by its negative (this yields an orientation of the edges of X, and thus the term 'oriented'). The *Laplacian matrix* of X is defined as

$$L(X) = D(X) - A(X) = CC^T,$$

while the *signless Laplacian matrix* of X is defined as

$$Q(X) = D(X) + A(X) = BB^T.$$

A *generalised adjacency matrix* of X is of the form

$$\alpha D(X) + A(X), \quad \alpha \in \mathbb{R}.$$

If the context is clear, then we simply write $A = A(X)$, $D = D(X)$, $L = L(X)$, and $Q = Q(X)$. If X is weighted k-regular, then $\alpha D + A = \alpha kI + A$, and so in this case, any generalised adjacency matrix of X is a translate of the adjacency matrix. Since $A = 0D + A$, $-L = -D + A$ and $Q = D + A$, we may view and analyze A, L, Q as a generalised adjacency matrix of X. Moreover, it is well-known that A is irreducible if and only if X is connected. Since D is diagonal, it follows that $\alpha D + A$ is irreducible if and only if X is connected. Note that $\alpha D + A$ is a real symmetric matrix that respects the adjacencies in X for all $\alpha \in \mathbb{R}$.

Let M be an irreducible nonnegative matrix. For any two vertices u and v in X, there is a positive integer $k := k(u, v)$ such that $(M^k)_{u,v} > 0$. If we further assume that $M = A$ and $u \neq v$, then the least such integer k is called the *distance* between vertices u and v in X, denoted $\operatorname{dist}(u, v)$. The *eccentricity* of vertex u in X is equal to $\max_{v \in V(X)} \operatorname{dist}(u, v)$, which is the maximum distance between u and any other vertex v in X. On the other hand, the *diameter* of X is equal to $\max_{u,v \in V(X)} \operatorname{dist}(u, v)$, which is the maximum eccentricity of a vertex in X (i.e., the farthest distance between any two vertices in X). For the case where X is unweighted, then $(A^k)_{u,v}$ is the number of walks of length k from u to v and $(A^k)_{u,u}$ is the number of closed walks starting at vertex u. In particular, $(A^2)_{u,u}$ is the number of edges incident with u (so that $(A^2)_{u,u} = \deg u$), while $(A^2)_{u,v}$ is the number of common neighbours of u and v.

Now, suppose X is an undirected connected weighted graph on n vertices, and M be a real symmetric that respects the adjacencies in X. Then we may order its eigenvalues in the following manner $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_n$. If $M = \alpha D + A$ and $\alpha \geq 0$, then M is an irreducible nonnegative matrix, and so by the Perron-Frobenius Theorem, $\lambda_1 > 0$ and $\alpha D + A$ has an all positive eigenvector associated with λ_1. This applies to A and Q, but not to L, since it is not a nonnegative matrix.

By definition, L and Q are positive semidefinite. In particular, if $M = L$, then it is known that $\lambda_1 = 0$ with associated eigenvector $\mathbf{1}$, and the multiplicity of 0 as an eigenvalue of L is equal to the number of components of X. Consequently, λ_1 is a simple eigenvalue if and only if X is a connected graph. Moreover, if X is connected and unweighted, then the *Matrix-Tree Theorem* says that the product of all nonzero eigenvalues of L divided by n is equal to the number of spanning trees in X [20].

Let X be a simple graph with at least one edge. In this case, A is a hollow matrix, and so the trace of A is zero. Now, because the largest eigenvalue of A is positive, it follows that A has a negative eigenvalue. Thus, A is not positive semidefinite (unlike L and Q). In particular, the condition that $\lambda_1 = -\lambda_n$ is equivalent to X being bipartite, and is also equivalent to the condition that the multiset of eigenvalues of A is closed under multiplication of -1.

We also define the notion of twin vertices in a weighted graph. Two vertices u and v in a weighted graph X are *twins* if

$$N_X(u)\backslash\{u,v\} = N_X(v)\backslash\{u,v\}$$

and the edges $\{u,w\}$ and $\{v,w\}$ have the same weight for all $w \in N_X(u)\backslash\{u,v\}$. A maximal subset $T = T(\eta)$ of $V(X)$ is a *twin set* in X if the vertices in T are pairwise twins and every pair of vertices in T are joined by an edge of weight $\eta \geq 0$. Twin vertices u and v are said to be *false twins* (also known as *open twins*) if they are non-adjacent (in which case $\eta = 0$), and *true twins* (also known as *closed twins*) otherwise (in which case $\eta \neq 0$). If X is unweighted, then $\eta \in \{0,1\}$. A twin set consisting of false twins is called a *false twin set*, and a *true twin set* otherwise. As an example, the vertex set of K_n is a true twin set, while a partite set of K_{n_1,n_2} with $n_1, n_2 \geq 2$ is a false twin set.

A spectral characterisation of twins is known [74, Lemma 2.9].

Lemma 2.2.1. *Let $T = T(\eta)$ be a twin set in X and let $u \in T$. Then $v \in T\backslash\{u\}$ if and only if $\mathbf{e}_u - \mathbf{e}_v$ is an eigenvector for the eigenvalue $\theta = \alpha \deg(u) - \eta$ of $\alpha D + A$.*

2.3 Algebra and number theory

This section contains facts from algebra and number theory that are useful later on.

Let M be an $n \times n$ complex matrix. The *exponential* e^M of the matrix M is defined as the power series

$$e^M = \sum_{j=0}^{\infty} \frac{1}{j!} M^j \tag{2.3.1}$$

where $M^0 = I$. From the above equation, it is immediate that

$$e^{(M^*)} = (e^M)^* \quad \text{and} \quad e^{(M^T)} = (e^M)^T.$$

Thus, e^M is Hermitian (resp., symmetric) whenever M is. Moreover, if M and N are commuting matrices, then

$$e^{M+N} = e^M e^N.$$

It is known that each $n \times n$ Hermitian matrix has real spectrum with an orthonormal set of eigenvectors that forms a basis for $\mathbb{C}^n$. In particular, a real symmetric matrix has an orthonormal set of eigenvectors that forms a basis for $\mathbb{R}^n$. This is the well-known spectral theorem for Hermitian matrices [55, 59], which we state below.

Theorem 2.3.1 (Spectral Decomposition). *Let M be an $n \times n$ Hermitian matrix. Then we can write*

$$M = \sum_{\lambda \in \operatorname{spec}(M)} \lambda E_\lambda, \tag{2.3.2}$$

where each E_λ is the orthogonal projection matrix onto the eigenspace associated with the eigenvalue λ. Moreover, the following conditions hold.

1. $E_\lambda^* = E_\lambda$, $E_\lambda^2 = E_\lambda$ *and* $E_\lambda E_\theta = 0$ *for all* $\lambda \neq \theta$.
2. $\displaystyle\sum_{\lambda \in \operatorname{spec}(M)} E_\lambda = I_n$.
3. *If g is an analytic function defined at each eigenvalue of M, then*

$$g(M) = \sum_{\lambda \in \operatorname{spec}(M)} g(\lambda) E_\lambda.$$

We refer to the matrices E_λ in Theorem 2.3.1 as *spectral idempotents*. When using indices, we use E_j to denote the spectral idempotent corresponding to λ_j. To find E_λ, simply choose any orthonormal basis $\{\mathbf{w}_1, \dots, \mathbf{w}_\ell\}$ for the eigenspace corresponding to λ, and set $E_\lambda = \sum_{j=1}^{\ell} \mathbf{w}_j \mathbf{w}_j^T$. For this reason, M and $M + tI$ have the same set of spectral idempotents. Moreover, if M is real symmetric, then each E_λ may be chosen to be real symmetric. Since $\alpha D + A$ is real symmetric, it admits a spectral decomposition for all $\alpha \in \mathbb{R}$, where all spectral idempotents are real symmetric.

Proposition 2.3.2. *Each spectral idempotent of a Hermitian matrix M is a polynomial in M with real coefficients.*

Proof. Assume M has spectral decomposition given in (2.3.2). Fix $\lambda \in \operatorname{spec}(M)$. Let $p(x)$ be a polynomial with real coefficients such that $p(\theta) = 0$ for all $\theta \in \operatorname{spec}(M)\backslash\{\lambda\}$ and $p(\lambda) = 1$. Invoking Theorem 2.3.1(3), we conclude that $p(M) = E_\lambda$. □

We will also need the well-known Cauchy-Schwarz inequality.

Theorem 2.3.3. *Let $\mathbf{x}$ and $\mathbf{y}$ be two vectors in $\mathbb{C}^n$. Then*

$$|\mathbf{x}^*\mathbf{y}| \leq \|\mathbf{x}\| \cdot \|\mathbf{y}\|$$

with equality if and only if $\mathbf{x}$ and $\mathbf{y}$ are linearly dependent over $\mathbb{C}$.

Next, we recall some algebraic and number theoretic concepts. An integer Δ is *square-free* if it is not divisible by a perfect square other than 1. For a prime p, the *p-adic valuation* of an integer $a \neq 0$, denoted $\nu_p(a)$, is the largest power of p that divides a. It is known that every integer $a \neq 0$ can be uniquely written as $a = 2^{\nu_2(a)}\ell$, where ℓ is an odd number. We adopt the convention that $\nu_p(0) = +\infty$ so that $\nu_p(0) > \nu_p(a)$ for any integer $a \neq 0$. An *algebraic number* $\lambda \in \mathbb{C}$ is a root of an irreducible polynomial $p(x)$ over $\mathbb{Q}$. If we also assume that $p(x)$ is monic, then we say that λ is an *algebraic integer*, while if $p(x)$ has degree two, then we say that λ is a *quadratic irrational.* Further, if $p(x)$ is both monic and degree two, then λ is a *quadratic integer.* Lastly, we say that $a, b \in \mathbb{R}$ are congruent modulo $c \in \mathbb{R}$, written as $a \equiv b \pmod{c}$, if $a = b + kc$ for some integer k.

We also define the following concept that is important throughout this work.

Definition 2.3.4. A set $S \subseteq \mathbb{R}$ with $|S| \geq 2$ satisfies the *ratio condition* if

$$\frac{\lambda - \theta}{\alpha - \beta} \in \mathbb{Q} \tag{2.3.3}$$

for any $\lambda, \theta, \alpha, \beta \in S$ with $\alpha \neq \beta$.

If all elements in S are rationals, then the ratio condition holds. The ratio condition also automatically holds whenever $|S| = 2$. For the case $|S| \geq 3$, Godsil characterised the sets S of real algebraic integers closed under taking algebraic conjugates that satisfy the ratio condition [37, Theorem 7.6.1]. Baptista and Coutinho observed that any set of algebraic numbers can be scaled with a common factor to obtain a set of algebraic integers [34]. Thus, we may restate [37, Theorem 7.6.1] as:

Theorem 2.3.5. *Let $r \geq 3$ and suppose $S = \{\lambda_1, \ldots, \lambda_r\}$ is a set of real algebraic numbers, closed under taking algebraic conjugates. Then S satisfies the ratio condition if and only if either of the following holds.*

1. *All elements in S are rationals.*
2. *All elements in S are quadratic irrationals. Moreover, there is a square-free integer $\Delta > 1$ and rationals $a, b_1, \ldots, b_r$ such that $\lambda_j = \frac{1}{2}(a + b_j\sqrt{\Delta})$.*

Additionally, if S is a set of real algebraic integers, then we may replace the terms 'rationals' and 'irrationals' by 'integers' in conditions 1 and 2.

3

Continuous quantum walks

A *continuous quantum walk* on a graph X is determined by the *transition matrix*

$$U_M(t) := e^{\mathrm{i}tM}, \quad t \in \mathbb{R}, \tag{3.0.1}$$

where $\mathrm{i}^2 = -1$ and M is a real symmetric matrix called the *Hamiltonian* associated with X. The matrix M is indexed by the vertices of X such that $M_{u,v} = 0$ if and only if there is no edge between u and v in X. In general, a Hamiltonian associated with a graph can be taken to be any Hermitian matrix that respects the adjacencies of the graph. In this work, we are mainly concerned with the case when M is an irreducible real symmetric matrix. The irreducibility condition on M is equivalent to the underlying graph X being connected. Throughout, if a result applies to any real symmetric matrix M, or if the Hamiltonian M is clear from the context, then we simply write $U_M(t)$ as $U(t)$. Often, we take M to be a generalised adjacency matrix $\alpha D + A$ of X (specifically, the adjacency matrix A or the Laplacian matrix L, and sometimes the signless Laplacian Q of X). But unless otherwise stated, our results apply to any irreducible real symmetric matrix M that respects the adjacencies of X. For simplicity, if we take M to be $\alpha D + A$, then we make the following assumption:

If $M = \alpha D + A$, then we further assume that X is simple (i.e., X is loopless).

The above assumption implies that $A(X)$ is a hollow matrix.

Our main goal in this section is to introduce the notion of quantum state transfer on pure states and establish basic results about fundamental concepts in continuous quantum walks, like eigenvalue supports, periodicity, and strong cospectrality. We also investigate quantum walks whose transition matrices can be built using the transition matrices of smaller quantum walks. A classic example of such a quantum walk is a physical system modelled by Cartesian products graphs, which can be viewed as a composite system of the underlying graphs.

3.1 Transition matrix

Let M be a Hamiltonian associated with X. The properties of matrix exponential yield the following properties of $U(t)$:

$$U_M(t_1+t_2) = U_M(t_1)U_M(t_2) \quad \text{for all } t_1, t_2 \in \mathbb{R}$$

and

$$U_M(-t) = U_M(t)^{-1} = U_M(t)^* = \overline{U_M(t)}^T = \overline{U_M(t)} \quad \text{for all } t. \tag{3.1.1}$$

Using the definition of exponential of a matrix, we may write (3.0.1) as

$$U_M(t) = \sum_{j=0}^{\infty} \frac{(\mathrm{i}t)^j}{j!} M^j. \tag{3.1.2}$$

Since M is real symmetric, the above equation implies that $U_M(t)$ is a complex symmetric matrix. Moreover, since $\mathrm{i}tM$ is skew-symmetric for each $t \in \mathbb{R}$, $U_M(t)$ is a unitary matrix for each $t \in \mathbb{R}$. Indeed, since M and $-M$ commute and $e^0 = I$, we obtain

$$U_M(t)U_M(t)^* = e^{\mathrm{i}tM}e^{-\mathrm{i}tM} = e^{\mathrm{i}t0} = I.$$

Proposition 3.1.1. *The transition matrix $U_M(t)$ of the quantum walk on X relative to M is a complex symmetric unitary matrix for all $t \in \mathbb{R}$.*

If we assume that M has spectral decomposition given in (2.3.2), then Theorem 2.3.1(3) also allows us to write $U(t)$ as

$$U(t) \;=\; \sum_{\lambda \in \operatorname{spec}(M)} e^{\mathrm{i}t\lambda} E_\lambda, \quad t \in \mathbb{R}. \tag{3.1.3}$$

Since M is real symmetric, each spectral idempotent E_λ is also real symmetric. Thus, equations (3.1.2) and (3.1.3) provide two distinct expressions for $U(t)$. The following examples illustrate how to obtain $U(t)$ using these two expressions.

Example 3.1.2. Let $M = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$, which may be viewed as the adjacency matrix of K_2. Observe that all even k and odd ℓ, we have

$$M^k = I \quad \text{and} \quad M^\ell = M.$$

Therefore,

$$U(t) = \sum_{j=0}^{\infty} \frac{(\mathrm{i}t)^j}{j!} M^j = \sum_{j=0}^{\infty} \frac{(\mathrm{i}t)^{2j}}{(2j)!} M^{2j} + \sum_{j=0}^{\infty} \frac{(\mathrm{i}t)^{2j+1}}{(2j+1)!} M^{2j+1} = I\cos t + \mathrm{i}M\sin t. \tag{3.1.4}$$

Example 3.1.3. Consider the adjacency matrix A of the complete graph K_n. We have $A = J - I$, and so $\operatorname{spec}(A) = \{n-1, -1\}$. An eigenvector for $\lambda_1 = n-1$ is $\mathbf{1}$, while $\{\mathbf{e}_1 - \mathbf{e}_2, \ldots, \mathbf{e}_1 - \mathbf{e}_n\}$ is a linearly independent set of eigenvectors for $\lambda_2 = -1$. This gives us

$$E_1 = \frac{1}{n}J \quad \text{and} \quad E_2 = I - \frac{1}{n}J.$$

Thus, the spectral decomposition of A is given by

$$A = (1)\frac{1}{n}J + (-1)\left(I - \frac{1}{n}\right)J. \tag{3.1.5}$$

and so we obtain $U_A(t) = e^{\mathrm{i}(n-1)t}E_1 + e^{-\mathrm{i}t}E_2$. Equivalently,

$$U_A(t) = e^{-\mathrm{i}t}\left((e^{\mathrm{i}tn} - 1)\frac{1}{n}J + I\right). \tag{3.1.6}$$

In particular, if $n = 2$, then A and the matrix M in Example 3.1.2 are equal. Thus, (3.1.4) and (3.1.6) yield the same transition matrix for K_2 relative to A given by

$$U(t) = \begin{bmatrix} \cos t & \mathrm{i}\sin t \\ \mathrm{i}\sin t & \cos t \end{bmatrix}. \tag{3.1.7}$$

In Example 3.1.2, the powers of M are equal to either M itself or the identity matrix, and so it was convenient to use (3.1.2) to obtain $U(t)$. But in general, notice that the sum in (3.1.3) is finite, whereas it is infinite in (3.1.2). Moreover, the sum in (3.1.3) follows immediately from the spectral decomposition of M. For these reasons, (3.1.3) is more convenient to utilise in obtaining an expression for $U(t)$.

3.2 Pure states

A *quantum state* is represented by a positive semidefinite matrix with trace one, known as a *density matrix*. If the initial state of our quantum walk on X relative to M is represented by a density matrix D, then according to [52], the state $D(t)$ at time t in X relative to M is given by

$$D(t) = U_M(t) D U_M(-t), \tag{3.2.1}$$

A density matrix D is a *pure state* if the rank of D is one, and it is a *real state* if all its entries are real. A pure state D can be written as $D = \frac{1}{\|\mathbf{x}\|^2}\mathbf{x}\mathbf{x}^*$ for some nonzero vector $\mathbf{x} \in \mathbb{C}^n$, where $\|\cdot\|$ is the Euclidean norm on $\mathbb{C}^n$. Thus, we abuse terminology and also refer to the complex vector $\mathbf{x}$ as a pure state. Technically, pure states are represented by unit complex vectors, but for our purposes, we consider each nonzero vector in the span of a single unit complex vector $\mathbf{v}$ to be the same pure state as $\mathbf{v}$. Consequently, we use the terms 'pure states' and 'nonzero complex vectors' interchangeably throughout this work. In particular, for each $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$, we let

$$D_{\mathbf{x}} := \frac{1}{\|\mathbf{x}\|^2}\mathbf{x}\mathbf{x}^*$$

denote the pure state associated with $\mathbf{x}$.

If u and v are vertices in X and $s \in \mathbb{C}\backslash\{0\}$, then a pure state of the form $\mathbf{x} = \mathbf{e}_u$ is called a *vertex state*, while $\mathbf{x} = \mathbf{e}_u + s\mathbf{e}_v$ is called an *s-pair state* [64]. In particular, a (-1)-pair state is called a *pair state* and a 1-pair state is called a *plus state*. Note that vertex, plus and pair states are real pure states, while $\mathbf{e}_u + s\mathbf{e}_v$ is a pure state that is not real whenever $s \in \mathbb{C}\backslash\mathbb{R}$.

The *mixing matrix* of the quantum walk on X relative to M is defined as

$$U_M(t) \circ U_M(-t) \quad \text{for all } t,$$

where $A \circ B$ denotes the Schur product of matrices A and B. Since $U(t)$ is unitary for each $t \in \mathbb{R}$ by Proposition 3.1.1, we have

$$\sum_{j=1}^{n} |U(t)_{u,j}|^2 = 1.$$

Now because $0 \leq |U(t)_{u,j}|^2 \leq 1$ for each j, the above sum allows us to interpret $|U(t)_{u,v}|^2$ as the probability that the vertex state $\mathbf{e}_u$ is transmitted to the vertex state $\mathbf{e}_v$ at time τ. By virtue of (3.1.1), we get that the mixing matrix is a symmetric doubly stochastic matrix whose entries that contains all probabilities of transfer between vertex states. In particular, the mixing matrix is a unistochastic matrix, since its entries are absolute values squared of a unitary matrix.

Now, let $\mathbf{x} \in \mathbb{C}^n \backslash \{0\}$. If $D_{\mathbf{x}}$ is the initial state of our quantum walk relative to M, then from (3.2.1), the state at time t is given by

$$D(t) = U_M(t) D_{\mathbf{x}} U_M(-t) = (U_M(t)\mathbf{x})(U_M(t)\mathbf{x})^*.$$

Now, if $\mathbf{y} \in \mathbb{C}^n$ with $\|\mathbf{x}\| = \|\mathbf{y}\|$, then Cauchy-Schwarz inequality gives us

$$\frac{1}{\|\mathbf{x}\|^2} |\mathbf{y}^* U_M(\tau)\mathbf{x}| \leq \frac{1}{\|\mathbf{x}\|^2} (|\mathbf{y}| \cdot |U_M(\tau)\mathbf{x}|) = \frac{1}{\|\mathbf{x}\|^2} (|\mathbf{x}| \cdot |\mathbf{x}|) = 1, \tag{3.2.2}$$

with equality if and only if $\{U_M(\tau)\mathbf{x}, \mathbf{y}\}$ is a linearly dependent set over $\mathbb{C}^n$.

Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ with $\|\mathbf{x}\| = \|\mathbf{y}\|$. The *fidelity* of quantum state transfer from $\mathbf{x}$ to $\mathbf{y}$ relative to the Hamiltonian M at time τ is defined as

$$\left(\frac{1}{\|\mathbf{x}\|^2} |\mathbf{y}^* U_M(\tau)\mathbf{x}| \right)^2, \tag{3.2.3}$$

which is a real number between 0 and 1 by (3.2.2). In particular, if $\mathbf{x} = \mathbf{e}_u$ and $\mathbf{y} = \mathbf{e}_v$, then

$$\left(\frac{1}{\|\mathbf{x}\|^2} |\mathbf{y}^* U(\tau)\mathbf{x}| \right)^2 = |U(t)_{u,v}|^2,$$

and so we may, in general, interpret the quantity in (3.2.3) as the probability that the pure state $\mathbf{x}$ is transmitted to the pure state $\mathbf{y}$ at time τ.

Two continuous quantum walks, one relative to the Hamiltonian M_1 and the other relative to M_2, are *equivalent* if their mixing matrices are equal up to some scalar multiple of t. That is, equivalent quantum walks have transition matrices whose corresponding entries are equal in modulus up to time dilation and time reversal. Since the entries of the mixing matrix are probabilities of transfer between vertex states, equivalent quantum walks exhibit the same behaviour. For instance, the quantum walks relative to the Hamiltonians M and $aI + bM$ for some $a, b \in \mathbb{R}$ are equivalent because

$$U_{aI+bM}(t) = e^{\mathrm{i}t(aI+bM)} = e^{\mathrm{i}ta} U_M(bt)$$

and so $|U_{aI+bM}(t)_{u,v}|^2 = |U_M(bt)_{u,v}|^2$ for all t and for all indices u and v. Here, b is the *dilation factor*, and there is *time reversal* if $b < 0$. In particular, if X is a weighted k-regular graph, then the quantum walks relative to the Hamiltonians $\alpha D + A$ and A are equivalent for all $\alpha \in \mathbb{R}$. In particular, this means that the quantum walks relative to A, L and Q are all equivalent for weighted-regular graphs.

3.3 Eigenvalue supports

Definition 3.3.1. The *eigenvalue support* of a vector $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ (in X relative to M), denoted $\Phi_{\mathbf{x}}(M)$, is the set

$$\Phi_{\mathbf{x}}(M) = \{\lambda \in \operatorname{spec}(M) : E_\lambda \mathbf{x} \neq \mathbf{0}\}.$$

If $|\Phi_{\mathbf{x}}| = 1$, then $\mathbf{x}$ is a *fixed state* relative to M.

If M is clear from the context, then we write $\Phi_{\mathbf{x}}(M)$ as $\Phi_{\mathbf{x}}$ for brevity.

Note that $\Phi_{\mathbf{x}}$ is always nonempty. Otherwise, $E_\lambda \mathbf{x} = \mathbf{0}$ for all $\lambda \in \operatorname{spec}(M)$, which happens if and only if $\mathbf{x} = \mathbf{0}$, a contradiction. Moreover, observe that

$$U(t)\mathbf{x} \;=\; \sum_{\lambda \in \operatorname{spec}(M)} e^{\mathrm{i}t\lambda} E_\lambda \mathbf{x} \;=\; \sum_{\lambda \in \Phi_{\mathbf{x}}} e^{\mathrm{i}t\lambda} E_\lambda \mathbf{x}, \tag{3.3.1}$$

and so the elements of $\Phi_{\mathbf{x}}$ are precisely those eigenvalues whose corresponding eigenspaces contribute to the propagation of the complex vector $\mathbf{x}$ relative to M.

The next propositions will be useful in the later sections. They are extensions of Propositions 1 and 3 in [53], respectively.

Proposition 3.3.2. *Let* $\mathbf{x} \in \mathbb{C}^n$. *If* $\varnothing \neq S \subseteq \operatorname{spec}(M)$, *then* $\Phi_{\mathbf{x}} = S$ *if and only if* $\mathbf{x} = \sum_{\lambda \in S} \mathbf{u}_\lambda$, *where each* $\mathbf{u}_\lambda$ *is an eigenvector for* M *associated with* $\lambda \in S$. *Additionally, if* $\mathbf{x}$ *is a real vector, then* $\mathbf{u}_\lambda$ *can be taken to be a real vector.*

Proof. Let $\Phi_{\mathbf{x}} = S$. If $\lambda \in S$, then $ME_\lambda \mathbf{x} = \lambda E_\lambda \mathbf{x}$, and so $\mathbf{u}_\lambda := E_\lambda \mathbf{x} \neq \mathbf{0}$ is an eigenvector for M associated with the eigenvalue λ. As the E_λ's sum to the identity, we get $\mathbf{x} = I\mathbf{x} = \sum_{\lambda \in S} E_\lambda \mathbf{x} = \sum_{\lambda \in S} \mathbf{u}_\lambda$. For the converse, let $\varnothing \neq S \subseteq \operatorname{spec}(M)$ and suppose $\mathbf{x} = \sum_{\lambda \in S} \mathbf{u}_\lambda$. Then $E_\theta \mathbf{x} = \sum_{\lambda \in S}(E_\theta \mathbf{u}_\lambda) \neq \mathbf{0}$ if and only if $\theta \in S$, and so $\Phi_{\mathbf{x}} = S$. The second statement follows from the fact that the E_λ's are real. □

Proposition 3.3.3. *The following are equivalent.*

1. *A vector* $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ *is a fixed state relative to* M.
2. *The set* $\Phi_{\mathbf{x}}$ *is a singleton set and* $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ *is an eigenvector for* M *associated with the lone eigenvalue* θ *in* $\Phi_{\mathbf{x}}$.
3. *For each* $t \in \mathbb{R}$, *we have* $U(t)\mathbf{x} = e^{\mathrm{i}t\theta}\mathbf{x}$.

Proof. The equivalence of 1 and 2 follows from Proposition 3.3.2, where we take S to be a singleton set. From (3.3.1), we have $U(t)\mathbf{x} = e^{\mathrm{i}t\theta}\mathbf{x}$ holds for all $t \in \mathbb{R}$ if and only if $\Phi_{\mathbf{x}} = \{\theta\}$ and $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ is an eigenvector for M associated with the eigenvalue θ. This proves the equivalence of 2 and 3. □

Example 3.3.4. For K_2, (3.1.7) gives us $U(t)(\mathbf{e}_1+\mathbf{e}_2) = e^{\mathrm{i}t}(\mathbf{e}_1+\mathbf{e}_2)$ for all t. Invoking Proposition 3.3.3, we get that the plus state $\mathbf{e}_1+\mathbf{e}_2$ is a fixed state relative to A. The pair state $\mathbf{e}_1-\mathbf{e}_2$ is also fixed in K_2. Indeed, these vectors are eigenvectors for $A(K_2)$ associated with the eigenvalue 1 and -1, respectively.

Example 3.3.5. If X is simple and either X is weighted-regular and $M \in \{A, L\}$, or $M = L$, then $\mathbf{x} \in \operatorname{span}\{\mathbf{1}\}\backslash\{\mathbf{0}\}$ is a fixed pure state in X. Moreover, if $\mathbf{v}$ is a Perron eigenvector for $M = A$, then $\mathbf{x} \in \operatorname{span}\{\mathbf{v}\}\backslash\{\mathbf{0}\}$ a fixed pure state in X.

We close this section with the following observation.

Lemma 3.3.6. *Let M be an irreducible matrix. If $\varnothing \neq S \subsetneq V(X)$, then*

$$\left(\bigcup_{u\in S}\Phi_{\mathbf{e}_u}\right)\bigcap\left(\bigcup_{v\in V(X)\backslash S}\Phi_{\mathbf{e}_v}\right)\neq\varnothing.$$

Proof. Suppose otherwise. Then for all $\lambda \in \bigcup_{u\in S}\Phi_{\mathbf{e}_u}$, we have $E_\lambda \mathbf{e}_v = 0$ for all $v \in V(X)\backslash S$, while for all $\theta \in \bigcup_{v\in V(X)\backslash S}\Phi_{\mathbf{e}_v}$, we have $E_\theta \mathbf{e}_u = 0$ for all $u \in S$. This implies that each spectral idempotent E_λ of M is block diagonal of the form $\begin{bmatrix} \mathcal{E}_\lambda & 0 \\ 0 & \mathcal{F}_\lambda \end{bmatrix}$, where each $\mathcal{E}_\lambda$ is $|S|$-by-$|S|$ and $\mathcal{F}_\lambda = 0$ whenever $\lambda \in \bigcup_{u\in S}\Phi_{\mathbf{e}_u}$, and $\mathcal{E}_\lambda = 0$ otherwise. This implies that M block diagonal, a contradiction to the irreducibility of M. $\square$

We close this section with a result obtained from adapting the proof of [64, Proposition 2.4].

Lemma 3.3.7. *Let $\mathbf{x} \in \mathbb{R}^n$. If $a\mathbf{x}$ has rational entries for some nonzero $a \in \mathbb{R}$ and* $\operatorname{spec}(M)$ *is closed under taking algebraic conjugates, then $\Phi_{\mathbf{x}}$ is closed under taking algebraic conjugates.*

Remark 3.3.8. Suppose $\phi(M,t)$ has rational coefficients. Then $\operatorname{spec}(M)$ is closed under taking algebraic conjugates and all elements of $\operatorname{spec}(M)$ are quadratic irrationals. Additionally, if $\phi(M,t)$ has integer coefficients, then all elements of $\operatorname{spec}(M)$ are quadratic integers. Furthermore, if $a\mathbf{x}$ has rational entries for some $a \neq 0$, then $\Phi_{\mathbf{x}}$ is closed under taking algebraic conjugates.

3.4 Weak cospectrality

Here, we extend the classical notion of cospectrality to what we call weak cospectrality, and provide a characterisation of this property.

Definition 3.4.1. Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ be linearly independent vectors with $\|\mathbf{x}\| = \|\mathbf{y}\|$. We say that $\mathbf{x}$ and $\mathbf{y}$ are *weakly cospectral* (in X relative to M) if for each $\lambda \in \Phi_{\mathbf{x}}$,

$$\mathbf{x}^* E_\lambda \mathbf{x} = \mathbf{y}^* E_\lambda \mathbf{y}. \tag{3.4.1}$$

Two vertices u and v in a graph are *cospectral* (in X relative to M) if the vectors $\mathbf{e}_u$ and $\mathbf{e}_v$ are weakly cospectral.

Remark 3.4.2. From the above definition, cospectrality of vertices u and v in X relative to M is equivalent to the condition that $(E_j)_{u,u} = (E_j)_{v,v}$ for each spectral idempotent j of M. Additionally, if $M = A$, then cospectrality of vertices u and v in X is equivalent to the condition that $\phi(A(X\backslash u), t) = \phi(A(X\backslash v), t)$, i.e., the vertex deleted subgraphs $X\backslash u$ and $X\backslash v$ are cospectral [56].

Note that weakly cospectral vectors have the same eigenvalue supports.

Lemma 3.4.3. *If* $\mathbf{x}$ *and* $\mathbf{y}$ *are weakly cospectral, then*

$$\mathbf{x}^* U(t) \mathbf{x} = \mathbf{y}^* U(t) \mathbf{y} \quad \text{for all } t \in \mathbb{R}.$$

Proof. Let $M = \sum_{\lambda \in \operatorname{spec}(M)} \lambda E_\lambda$ be the spectral decomposition of M. By assumption, we have $\mathbf{x}^* E_\lambda \mathbf{x} = \mathbf{y}^* E_\lambda \mathbf{y}$, and so

$$\mathbf{x}^* U(t) \mathbf{x} \; = \sum_{\lambda \in \operatorname{spec}(M)} e^{\mathrm{i}t\lambda} \mathbf{x}^* E_\lambda \mathbf{x} = \sum_{\lambda \in \operatorname{spec}(M)} e^{\mathrm{i}t\lambda} \mathbf{y}^* E_\lambda \mathbf{y} = \mathbf{y}^* U(t) \mathbf{y}$$

for all $t \in \mathbb{R}$. ☐

Remark 3.4.4. If vertices u and v in X are cospectral, then Lemma 3.4.3 implies that $U(t)_{u,u} = U(t)_{v,v}$ for all t.

Proposition 3.4.5. *If* $\mathbf{x}$ *and* $\mathbf{y}$ *are weakly cospectral, then so are* $\mathbf{x}$ *and* $\overline{\mathbf{y}}$.

Proof. By assumption, we have $\mathbf{x}^* E_\lambda \mathbf{x} = \mathbf{y}^* E_\lambda \mathbf{y}$ for each $\lambda \in \Phi_{\mathbf{x}}$. Since each E_j is positive semidefinite, $\mathbf{x}^* E_\lambda \mathbf{x}$ is real and nonnegative for each j, and therefore, we have $\mathbf{y}^* E_\lambda \mathbf{y} = \overline{(E_\lambda \mathbf{y})^* \mathbf{y}} = (E_\lambda \mathbf{y})^T \overline{\mathbf{y}} = \mathbf{y}^T E_j \overline{\mathbf{y}} = (\overline{\mathbf{y}})^* E_j \overline{\mathbf{y}}$. ☐

The following result characterises weak cospectrality. It can be viewed as an extension of [56, Theorem 3.1], from which we base our proof closely.

Theorem 3.4.6. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$*. The following are equivalent.*

1. $\mathbf{x}$ *and* $\mathbf{y}$ *are weakly cospectral.*

2. $\|E_\lambda \mathbf{x}\| = \|E_\lambda \mathbf{y}\|$ *for all* $\lambda \in \Phi_{\mathbf{x}}$*.*

3. $\mathbf{x}^* M^k \mathbf{x} = \mathbf{y}^* M^k \mathbf{y}$ *for all integers* $k \geq 0$*.*

Proof. Let $M = \sum_{\lambda \in \mathrm{spec}(M)} \lambda E_\lambda$ be the spectral decomposition of M. Since each spectral idempotent E_λ is real symmetric, we get

$$\mathbf{x}^* E_\lambda \mathbf{x} = \mathbf{x}^* E_\lambda^2 \mathbf{x} = \mathbf{x}^* E_\lambda^* E_\lambda \mathbf{x} = (E_\lambda \mathbf{x})^* E_\lambda \mathbf{x} = \|E_\lambda \mathbf{x}\| > 0$$

for all $\lambda \in \Phi_{\mathbf{x}}$. Thus, 1 and 2 are equivalent. Next, suppose $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral. Since $M^k = \sum_{\lambda \in \mathrm{spec}(M)} \lambda^k E_\lambda$, we get

$$\mathbf{x}^* M^k \mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \lambda^k \mathbf{x}^* E_\lambda \mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \lambda^k \mathbf{y}^* E_\lambda \mathbf{y} = \mathbf{y}^* M^k \mathbf{y}$$

for all integers $k \geq 0$. Conversely, suppose $\mathbf{x}^* M^k \mathbf{x} = \mathbf{y}^* M^k \mathbf{y}$ for all integers $k \geq 0$. For each $\lambda \in \Phi_{\mathbf{x}}$, Proposition 2.3.2 yields a polynomial $p_\lambda(x)$ with real coefficients such that $p_\lambda(M) = E_\lambda$. Hence, we may write $E_\lambda = \sum_{j=1}^q a_j M^j$ where each $a_j \in \mathbb{R}$. Thus, $\mathbf{x}^* E_\lambda \mathbf{x} = \mathbf{x}^* \left(\sum_{j=1}^q a_j M^j \right) \mathbf{x} = \sum_{j=1}^q a_j \mathbf{x}^* M^j \mathbf{x} = \sum_{j=1}^q a_j \mathbf{y}^* M^j \mathbf{y} = \mathbf{y}^* E_\lambda \mathbf{y}$. This proves the equivalence of 1 and 3. □

Corollary 3.4.7. *If* $P \neq I$ *is a permutation matrix satisfying* $M = P^T M P$ *and* $P\mathbf{x} = \mathbf{y}$*, then* $\mathbf{x}$ *and* $\mathbf{y}$ *are weakly cospectral.*

Proof. Since $P^T P = P P^T = I$ and $M = P^T M P$, we have $M^k = P^T M^k P$ for all integers $k \geq 0$. Thus, $\mathbf{x}^* M^k \mathbf{x} = (P\mathbf{y})^* M^k (P\mathbf{y}) = \mathbf{y}^* (P^T M^k P) \mathbf{y} = \mathbf{y}^* M^k \mathbf{y}$. Invoking Theorem 3.4.6 yields the desired conclusion. □

If $M = \alpha D + A$ and X has a nontrivial automorphism represented by a matrix P, then $P \neq I$ is a permutation matrix satisfying $M = P^T M P$. In this case, if $P\mathbf{x} = \mathbf{y}$, then Corollary 3.4.7 implies that $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral.

We give an example that illustrates Theorem 3.4.6.

Example 3.4.8. Let X be a graph. The following hold.

1. Let $M = \alpha D + A$. If P is a permutation matrix that represents a nontrivial automorphism of X that sends u to v (so that $P\mathbf{e}_u = \mathbf{e}_v$), then $\mathbf{e}_u$ and $\mathbf{e}_v$ are weakly cospectral by Corollary 3.4.7. In particular, if X is a vertex-transitive graph, then $\mathbf{e}_u$ and $\mathbf{e}_v$ are weakly cospectral for all vertices u and v in X.

2. Let $X = K_n$ and $M = A$. Note that $A = J - I$ and $J^\ell = n^{\ell-1}J$ for each integer $\ell \geq 1$. Since J and I commute, we have

$$A^k = (J - I)^k = \sum_{\ell=0}^{k} \binom{k}{\ell} J^\ell = I + \sum_{\ell=1}^{k} \binom{k}{\ell} n^{\ell-1} J.$$

   Assume $\mathbf{x}$ and $\mathbf{y}$ are linearly independent vectors in $\mathbb{C}^n$ satisfying $\|\mathbf{x}\| = \|\mathbf{y}\|$ and $\mathbf{1}^T\mathbf{x} = \zeta\mathbf{1}^T\mathbf{y} \neq 0$ for some unit complex number ζ. Since $J = \mathbf{1}\mathbf{1}^T$, we have $\mathbf{x}^* J\mathbf{x} = |\mathbf{1}^T\mathbf{x}|^2 = |\mathbf{1}^T\mathbf{y}|^2 = \mathbf{y}^* J\mathbf{y}$. Combining this with the above equation yields

$$\mathbf{x}^* A^k\mathbf{x} = \|\mathbf{x}\|^2 + \sum_{\ell=1}^{k} \binom{k}{\ell} n^{\ell-1}(\mathbf{x}^* J\mathbf{x}) = \|\mathbf{x}\|^2 + \sum_{\ell=1}^{k} \binom{k}{\ell} n^{\ell-1}(\mathbf{y}^* J\mathbf{y}) = \mathbf{y}^* A^k\mathbf{y}$$

   for all integers $k \geq 0$. Invoking Theorem 3.4.6(3), we get that $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral. This also applies to $M = \alpha D + A$ because K_n is regular.

The *walk module generated by a vector* $\mathbf{u} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ *relative to* M, denoted $W_M(\mathbf{u})$, is the subspace of $\mathbb{C}^n$ generated by the set $\{M^j\mathbf{u} : j = 0, 1, \ldots, n-1\}$. Such a subspace is M-invariant, and so we may view it as a module over $\mathbb{C}[M]$, the polynomials in M with complex coefficients.

The walk modules $W_M(\mathbf{x}+\mathbf{y})$ and $W_M(\mathbf{x}-\mathbf{y})$ are orthogonal if and only if $\langle M^j(\mathbf{x}+\mathbf{y}), M^\ell(\mathbf{x}-\mathbf{y})\rangle = 0$ for all integers $j, \ell \geq 0$, where $\langle\cdot,\cdot\rangle$ is the complex inner product. Equivalently, for all integers $j \geq 0$, we have

$$0 = (\mathbf{x}+\mathbf{y})^* M^j(\mathbf{x}-\mathbf{y}) = \mathbf{x}^* M^j\mathbf{x} - \mathbf{y}^* M^j\mathbf{y} + 2\operatorname{Im}(\mathbf{y}^* M^j\mathbf{x}) \tag{3.4.2}$$

The last result in this section generalises the equivalence of statements a and g in [56, Theorem 3.1].

Proposition 3.4.9. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ *be weakly cospectral. The subspaces* $W_M(\mathbf{x} + \mathbf{y})$ *and* $W_M(\mathbf{x} - \mathbf{y})$ *of* $\mathbb{C}^n$ *are orthogonal if and only if* $\operatorname{Im}\mathbf{y}$ *is in the orthogonal complement of* $W_M(\mathbf{x})$ *in* $\mathbb{C}^n$*.*

Proof. Let $\mathbf{y} = \operatorname{Re}\mathbf{y} + \mathrm{i}\operatorname{Im}\mathbf{y}$, where $\operatorname{Re}\mathbf{y}$ and $\operatorname{Im}\mathbf{y}$ are real vectors representing the real and imaginary parts of the components of $\mathbf{y}$. If $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral vectors, then by (3.4.2), $W_M(\mathbf{x}+\mathbf{y})$ and $W_M(\mathbf{x}-\mathbf{y})$ are orthogonal if and only if $\operatorname{Im}(\mathbf{y}^* M^j\mathbf{x}) = (\operatorname{Im}\mathbf{y})^T M^j\mathbf{x} = 0$. □

3.5 Strong cospectrality

One of the first papers on strong cospectrality between vertex states is due to Godsil [50], where it was shown that strong cospectrality is a necessary condition for perfect state transfer between vertex states. This prompted researchers to further explore the topic of strong cospectrality between vertex states [4, 33, 39]. On the other hand, m-strong cospectrality between vertex states was first introduced by Chan and Zhan in the context of discrete quantum walks [25]. Strong cospectrality between vertex states has also been studied in the context of pretty good state transfer [43, 83] and vertex sedentariness [76, 77]. These are two types of quantum state transfer that are outside of the scope of this thesis, but we nonetheless mention them to convince the reader that our exploration of strong cospectrality is well-motivated.

As we will show later, strong cospectrality in general is a necessary condition for two vectors to admit perfect state transfer. This motivates us in this section to develop the theory of strong cospectrality between pure states. We derive properties and characterizations of strong cospectrality that are useful in later sections. We also explore the notion of m-strong cospectrality in continuous quantum walks.

Definition 3.5.1. Suppose $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ are two linearly independent vectors with $\|\mathbf{x}\| = \|\mathbf{y}\|$. We say that $\mathbf{x}$ and $\mathbf{y}$ are *strongly cospectral* (in X relative to M) if for each $\lambda \in \Phi_{\mathbf{x}}$, there is a unit complex number ζ_λ such that

$$E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}. \tag{3.5.1}$$

We say that $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ are *m-strongly cospectral* if we can write each ζ_λ in (3.5.1) as $\zeta_\lambda = e^{\mathrm{i}2\pi\ell_\lambda/m}$ for some integer $\ell_\lambda \in \mathbb{Z}_m$ and $\gcd(\ell_\lambda, m) = 1$ for at least one $\lambda \in \Phi_{\mathbf{x}}$.

Strongly cospectral vectors have equal eigenvalue supports. Moreover, for m-strong cospectrality, at least one of the ζ_λ's in (3.5.1) is a primitive root of unity.

Remark 3.5.2. If $\mathbf{x}, \mathbf{y}$ are strongly cospectral, then there are at least two elements $\lambda, \theta \in \Phi_{\mathbf{x}}$ such that $\zeta_\lambda \neq \zeta_\theta$, and so $|\Phi_{\mathbf{x}}| \geq 2$. Otherwise, $\gamma = \zeta_\lambda$ for all $\lambda \in \Phi_{\mathbf{x}}$, which yields $\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} E_\lambda \mathbf{x} = \gamma \sum_{\lambda \in \Phi_{\mathbf{y}}} E_\lambda \mathbf{y} = \gamma \mathbf{y}$, a contradiction to the linear independence of $\mathbf{x}$ and $\mathbf{y}$. Furthermore, since $|\Phi_{\mathbf{x}}| \geq 2$, a fixed state is not involved in strong cospectrality by Proposition 3.3.3.

Remark 3.5.3. Let $d = |\Phi_{\mathbf{x}}|$. There are $m^{d-1} - 1$ vectors $\mathbf{y}$ that are m-strongly cospectral with $\mathbf{x}$. To see this, for a fixed $\lambda \in \Phi_{\mathbf{x}}$, one may pick an integer $\ell_\lambda \in \mathbb{Z}_m$ such that $\gcd(\ell_\lambda, m) = 1$. Then for the rest of $\theta \in \Phi_{\mathbf{x}} \backslash \{\lambda\}$, pick any $\ell_\theta \in \mathbb{Z}_m$.

This ensures that the ζ_λ in (3.5.1) are m-th roots of unity with at least one being primitive. This yields the count m^{d-1}, and because we want to leave out the case that all angles are equal, we subtract one. Thus, unlike the general complex case, there are only finitely many vectors that are m-strongly cospectral with $\mathbf{x}$.

Remark 3.5.4. If each $\zeta_\lambda = \pm 1$, then we may partition $\Phi_{\mathbf{x}}$ into two nonempty sets:

$$\Phi^+_{\mathbf{x},\mathbf{y}} := \{\lambda \in \Phi_{\mathbf{x}} : E_\lambda \mathbf{x} = E_\lambda \mathbf{y}\} \quad \text{and} \quad \Phi^-_{\mathbf{x},\mathbf{y}} := \{\lambda \in \Phi_{\mathbf{x}} : E_\lambda \mathbf{x} = -E_\lambda \mathbf{y}\}. \tag{3.5.2}$$

If $\mathbf{x}$ and $\mathbf{y}$ are real vectors that are strongly cospectral, then $\zeta_\lambda = \pm 1$ for each $\lambda \in \Phi_{\mathbf{x}}$. Thus, strong cospectrality between real vectors is simply 2-strong cospectrality.

If $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, then each ζ_λ in (3.5.1) is equal to ± 1 by Remark 3.5.4. In this case, we obtain the classical notion of strong cospectrality, a concept that appeared in [50, Lemma 11.1], and possibly earlier. It was later on studied in depth for vertex states by Godsil and Smith in [56]. On the other hand, the concept of m-strongly cospectrality was first coined by Chan and Zhan in their investigation of pretty good state transfer in discrete quantum walks [25].

Remark 3.5.5. Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ be strongly cospectral, so that $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ for each $\lambda \in \Phi_{\mathbf{x}}$. Fix $\lambda \in \Phi_{\mathbf{x}}$ and let $\mathbf{w}$ be an eigenvector for λ. Then $\mathbf{w}^* E_\lambda \mathbf{x} = \zeta_\lambda \mathbf{w}^* E_\lambda \mathbf{y}$, or equivalently, $(E_\lambda \mathbf{w})^* \mathbf{x} = \zeta_\lambda (E_\lambda \mathbf{w})^* \mathbf{y}$. Since $E_\lambda \mathbf{w} = \mathbf{w}$, we get

$$\mathbf{w}^* \mathbf{x} = \zeta_\lambda \mathbf{w}^* \mathbf{y}.$$

In particular, if $\mathbf{x}$ and $\mathbf{y}$ are 2-strongly cospectral, then $\zeta_\lambda = \pm 1$, in which case 2-strongly cospectrality between $\mathbf{x}$ and $\mathbf{y}$ is equivalent to the condition that for each $\lambda \in \Phi_{\mathbf{x}}$, either $\mathbf{w}^* \mathbf{x} = \mathbf{w}^* \mathbf{y}$ for each eigenvector $\mathbf{w}$ for λ, or $\mathbf{w}^* \mathbf{x} = -\mathbf{w}^* \mathbf{y}$ for each eigenvector $\mathbf{w}$ for λ. Additionally, if $\mathbf{x} = \mathbf{e}_u$ and $\mathbf{y} = \mathbf{e}_v$, then strongly cospectrality between $\mathbf{e}_u$ and $\mathbf{e}_v$ is equivalent to the condition that for each $\lambda \in \Phi_{\mathbf{x}}$, either the uth and vth entries of each eigenvector $\mathbf{w}$ for λ are equal, or the uth and vth entries of each eigenvector $\mathbf{w}$ for λ are opposite in signs.

Remark 3.5.6. Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ be strongly cospectral such that $\mathbf{x}$ is a real vector and $\mathbf{y}$ is a nonreal vector (that is, $\mathbf{y}$ has at least one non-real entry). Since each spectral idempotent E_λ is a real matrix, each $E_\lambda \mathbf{x}$ is a real vector. Now, if $\mathbf{x}, \mathbf{y}$ are 2-strongly cospectral, that is $E_\lambda \mathbf{x} = \pm E_\lambda \mathbf{y}$ for each $\lambda \in \Phi_{\mathbf{x}}$, then each $E_\lambda \mathbf{y}$ is necessarily a real vector, and so $\sum_{\lambda \in \Phi_{\mathbf{x}}} E_\lambda \mathbf{y} = \mathbf{y}$ is a real vector, a contradiction. Thus, $\mathbf{x}, \mathbf{y}$ are not 2-strongly cospectral. In other words, if $\mathbf{x}, \mathbf{y}$ are 2-strongly cospectral, then either both $\mathbf{x}, \mathbf{y}$ are real vectors, or they are both nonreal vectors.

The next result may be viewed as a generalisation of [56, Lemma 4.1].

Theorem 3.5.7. *The vectors* $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral if and only if they are weakly cospectral and* $E_\lambda \mathbf{x}$ *and* $E_\lambda \mathbf{y}$ *are parallel vectors for each* $\lambda \in \Phi_{\mathbf{x}}$.

Proof. Suppose $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral. By definition, the vectors $E_\lambda \mathbf{x}$ and $E_\lambda \mathbf{y}$ are parallel for each $\lambda \in \Phi_{\mathbf{x}}$. Moreover, we have $(E_j \mathbf{x})^*(E_j \mathbf{x}) = (E_j \mathbf{y})^*(E_j \mathbf{y})$ for all $\lambda \in \Phi_{\mathbf{x}}$. Hence $\mathbf{x}^* E_j \mathbf{x} = \mathbf{y}^* E_j \mathbf{y}$ for all $\lambda \in \Phi_{\mathbf{x}}$. That is, $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral. For the converse, suppose $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral, and $E_\lambda \mathbf{x}$ and $E_\lambda \mathbf{y}$ are parallel vectors for each $\lambda \in \Phi_{\mathbf{x}}$. The latter assumption implies that for each $\lambda \in \Phi_{\mathbf{x}}$, we have $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ for some $z_\lambda \in \mathbb{C}$. That is, for a fixed $\lambda \in \Phi_{\mathbf{x}}$, we have $\mathbf{w}^* \mathbf{x} = \zeta_\lambda \mathbf{w}^* \mathbf{y}$ for each eigenvector $\mathbf{w}$ associated with λ. If $\{\mathbf{w}_j\}$ is an orthonormal basis for the eigenspace of λ, then we may write $E_\lambda = \sum_j \mathbf{w}_j \mathbf{w}_j^*$, and so

$$\mathbf{x}^* E_\lambda \mathbf{x} = \textstyle\sum_j (\mathbf{w}_j^* \mathbf{x})^* (\mathbf{w}_j^* \mathbf{x}) = \sum_j (\zeta_\lambda \mathbf{w}_j^* \mathbf{y})^* (\zeta_\lambda \mathbf{w}_j^* \mathbf{y}) = |\zeta_\lambda|^2 \mathbf{y}^* E_\lambda \mathbf{y}.$$

Since $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral, the above equation yields $|\zeta_\lambda| = 1$. Equivalently, $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral. □

Corollary 3.5.8. *If all eigenvalues of* M *are simple, then the vectors* $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral if and only if they are weakly cospectral.*

Proof. Since each eigenspace of M has dimension one, we may write each E_λ as $\mathbf{w}\mathbf{w}^*$ for some unit vector $\mathbf{w}$. From this, it follows that $E_\lambda \mathbf{x}$ and $E_\lambda \mathbf{y}$ are parallel vectors for each $\lambda \in \Phi_{\mathbf{x}}$ and so the conclusion is immediate from Theorem 3.5.7. □

Proposition 3.5.9. *If* $\mathbf{x}$ *and* $\mathbf{y}$ *are weakly (resp., strongly) cospectral, then so are* $P\mathbf{x}$ *and* $P\mathbf{y}$ *for every permutation matrix* P *such that* $M = P^T M P$.

Proof. Follows from (3.4.1), (3.5.1) and the fact that $PE_\lambda = E_\lambda P$ for all $\lambda \in \Phi_{\mathbf{x}}$. □

We also extend [56, Corollary 6.4] to complex vectors.

Lemma 3.5.10. *Let* $\mathbf{x}$ *and* $\mathbf{y}$ *be strongly cospectral, and suppose* P *is a permutation matrix such that* $M = P^T M P$. *If* $P\mathbf{y} = \mathbf{y}$, *then* $P\mathbf{x} = \mathbf{x}$.

Proof. By assumption, P is a permutation matrix such that $M = P^T M P$. This implies that $PE_\lambda = E_\lambda P$ for each $\lambda \in \operatorname{spec}(M)$. Now, if $P\mathbf{y} = \mathbf{y}$, then we have

$$E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y} = \zeta_\lambda P^T E_\lambda P \mathbf{y} = \zeta_\lambda P^T E_\lambda \mathbf{y} = \zeta_\lambda \overline{\zeta_\lambda} P^T E_\lambda \mathbf{x} = P^T E_\lambda \mathbf{x}.$$

Since the E_λ's sum to the identity, the above equation yields $P\mathbf{x} = \mathbf{x}$. □

The above lemma implies that if $M = \alpha D + A$, then every automorphism of X that fixes $\mathbf{y}$ also fixes $\mathbf{x}$.

Example 3.5.11. Let u, v_1, v_2 be pairwise twin vertices in X. For $j \in \{1, 2\}$, there is an automorphism ψ_j that sends u to v_j and fixes all the vertices in $V(X)\backslash\{u, v_j\}$. Therefore, $\mathbf{e}_u$, $\mathbf{e}_{v_1}$ and $\mathbf{e}_{v_2}$ are pairwise weakly cospectral by Corollary 3.4.7. Since each ψ_j is an involution, it follows that ψ_j sends v_j to u. Thus, there is an automorphism ψ_1 that fixes v_2 but not v_1, and so $\mathbf{e}_{v_1}$ and $\mathbf{e}_{v_2}$ are not strongly cospectral by Lemma 3.5.10. In particular, this example implies that vertex states corresponding to a set of pairwise twin vertices with at least three elements are pairwise weakly cospectral, but no two of them are strongly cospectral.

We now provide a matrix-theoretic characterisation of strongly cospectral vectors, which extends [53, Theorem 19]. This will prove useful in the latter sections.

Theorem 3.5.12. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ *and suppose* $\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \mathbf{u}_\lambda$*, where each* $\mathbf{u}_\lambda$ *is an eigenvector associated with an eigenvalue* $\lambda \in \Phi_{\mathbf{x}}$*. Then* $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ *for each* $\lambda \in \Phi_{\mathbf{x}}$ *and for some unit complex number* ζ_λ *if and only if*

$$\mathbf{y} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \overline{\zeta_\lambda} \mathbf{u}_\lambda.$$

Proof. By Proposition 3.3.2, we may write $\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \mathbf{u}_\lambda$. If $\lambda \in \Phi_{\mathbf{x}}$, then we obtain $E_\lambda \mathbf{x} = \mathbf{u}_\lambda$. Thus, $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ if and only if $E_\lambda \mathbf{y} = \overline{\zeta_\lambda} \mathbf{u}_\lambda$. Equivalently,

$$\mathbf{y} = \sum_{\lambda \in \Phi_{\mathbf{y}}} E_\lambda \mathbf{y} = \sum_{\lambda \in \Phi_{\mathbf{y}}} \overline{\zeta_\lambda} \mathbf{u}_\lambda.$$

Thus, the above theorem holds. □

Remark 3.5.13. For $r \geq 2$, let $\Phi_{\mathbf{x}} = \{\lambda_1, \ldots, \lambda_r\}$. By Proposition 3.3.2, we may write $\mathbf{x} = \sum_{j=1}^r \mathbf{u}_j$, where $\mathbf{u}_j$ is an eigenvector associated with λ_j. For every r-tuple $(\zeta_1, \ldots, \zeta_r)$ of unit complex numbers such that $\zeta_\ell \neq \zeta_k$ for at least two indices ℓ, k, the vector $\mathbf{y} = \sum_{j=1}^r \overline{\zeta_j} \mathbf{u}_j$ is strongly cospectral with $\mathbf{x}$. Therefore, there are infinitely many complex vectors $\mathbf{y}$ that are strongly cospectral with $\mathbf{x}$.

Now, if $\mathbf{x}$ is strongly cospectral with $\mathbf{y} = \sum_{j=1}^r \overline{\zeta_j} \mathbf{u}_j$ and $\mathbf{z} = \sum_{j=1}^r \overline{\alpha_j} \mathbf{u}_j$, then it is not necessarily the case that $(\zeta_1, \ldots, \zeta_r)$ and $(\alpha_1, \ldots, \alpha_r)$ are linearly dependent. Equivalently, it need not happen that $\mathbf{y} = \eta \mathbf{z}$ for some unit complex number η.

In the following example, we illustrate Theorem 3.5.12 and provide an example of weakly cospectral vectors that are not strongly cospectral.

Example 3.5.14. Let $X = K_n$ and $M = A$. Then $\mathbf{1}$ is an eigenvector for M for the eigenvalue $n-1$, while $\mathbf{e}_1 - \mathbf{e}_j$ is an eigenvector for M for the eigenvalue -1 for each $j \in \{2, \ldots, n\}$. Let E_{n-1} and E_{-1} be the spectral idempotents associated with $n-1$ and -1. Assume $\mathbf{x}$ and $\mathbf{y}$ are linearly independent vectors in $\mathbb{C}^n$ satisfying $\|\mathbf{x}\| = \|\mathbf{y}\|$. The following hold.

1. If $\mathbf{x} = \mathbf{1} + (\mathbf{e}_1 - \mathbf{e}_2)$ and $\mathbf{y} = \overline{\zeta}\mathbf{1} + \overline{\zeta'}(\mathbf{e}_1 - \mathbf{e}_2)$ for some unit complex numbers ζ and ζ' with $\zeta \neq \zeta'$, then Theorem 3.5.12 implies that $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral with $E_{n-1}\mathbf{x} = \zeta E_{n-1}\mathbf{y}$ and $E_{-1}\mathbf{x} = \zeta' E_{-1}\mathbf{y}$.
2. If $\mathbf{x} = \mathbf{1} + (\mathbf{e}_1 - \mathbf{e}_2)$ and $\mathbf{y} = \zeta\mathbf{1} + \zeta'(\mathbf{e}_1 - \mathbf{e}_2) + (\mathbf{e}_1 - \mathbf{e}_3)$ for some unit complex numbers ζ, ζ' with $\zeta \neq \zeta'$, then $\mathbf{x}$ and $\mathbf{y}$ are not strongly cospectral because $\mathbf{y}$ does not have the desired form as in Theorem 3.5.12. However, we have $\mathbf{1}^T\mathbf{x} = \zeta\mathbf{1}^T\mathbf{y} \neq 0$, and so Example 3.4.8(2) implies that $\mathbf{x}$ and $\mathbf{y}$ are weakly cospectral. Thus, while strong cospectrality implies weak cospectrality by Theorem 3.5.7, the converse of this fact does not hold.

If $\mathbf{x} \in \mathbb{R}^n$, then $\overline{\mathbf{x}} = \mathbf{x}$. Thus, $\mathbf{x}$ and $\overline{\mathbf{x}}$ are linearly dependent, and so they are not strongly cospectral. For the case that $\mathbf{x} \in \mathbb{C}^n \backslash \mathbb{R}^n$, we have the following result.

Theorem 3.5.15. *Let $\mathbf{x} \in \mathbb{C}^n \backslash \mathbb{R}^n$. Then $\mathbf{x}$ and $\overline{\mathbf{x}}$ are strongly cospectral if and only if we can write*

$$\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} e^{\mathrm{i}\mu_\lambda}\mathbf{u}_\lambda \tag{3.5.3}$$

where each $\mu_\lambda \in [0, 2\pi)$ and each $\mathbf{u}_\lambda$ is a real eigenvector associated with $\lambda \in \Phi_{\mathbf{x}}$. In this case, $E_\lambda\mathbf{x} = e^{\mathrm{i}2\mu_\lambda}E_\lambda\overline{\mathbf{x}}$ for each $\lambda \in \Phi_{\mathbf{x}}$.

Proof. Let $\mathbf{x}$ and $\overline{\mathbf{x}}$ be strongly cospectral. Then we may write $\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \mathbf{w}_\lambda$ and $\overline{\mathbf{x}} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \overline{\zeta_\lambda}\mathbf{w}_\lambda$ by Theorem 3.5.12, where each $\mathbf{w}_\lambda$ is an eigenvector associated with an eigenvalue $\lambda \in \Phi_{\mathbf{x}}$. As $\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \mathbf{w}_\lambda = \sum_{\lambda \in \Phi_{\mathbf{x}}} \zeta_\lambda\overline{\mathbf{w}_\lambda}$, we obtain

$$E_\lambda\mathbf{x} = \mathbf{w}_\lambda = \zeta_\lambda\overline{\mathbf{w}_\lambda} \quad \text{for each } \lambda \in \Phi_{\mathbf{x}}.$$

Now, fix $\lambda \in \Phi_{\mathbf{x}}$. Since $\mathbf{w}_\lambda$ is an eigenvector for M and M is irreducible, it follows that $\mathbf{w}_\lambda$ has at least two nonzero entries, say $z_1, z_2 \in \mathbb{C}\backslash\{0\}$. Let μ_1 and μ_2 be the arguments of z_1 and z_2, respectively, where $\mu_1, \mu_2 \in [0, 2\pi)$. Since $\mathbf{w}_\lambda - \zeta_\lambda\overline{\mathbf{w}_\lambda} = 0$, we have $\zeta_\lambda = \frac{z_1}{\overline{z_1}} = \frac{z_2}{\overline{z_2}}$. Thus, $\zeta_\lambda = e^{\mathrm{i}2\mu_1} = e^{\mathrm{i}2\mu_2}$, and so $\mu_1 = \mu_2 := \mu_\lambda$ because $\mu_1, \mu_2 \in [0, 2\pi)$. Hence, all nonzero entries of $\mathbf{w}_\lambda$ have the same arguments modulo 2π, and so $\mathbf{w}_\lambda = e^{\mathrm{i}\mu_\lambda}\mathbf{u}_\lambda$ for some real vector $\mathbf{u}_\lambda$. The converse is straightforward. $\square$

Remark 3.5.16. If each $e^{\mathrm{i}\mu_\lambda}$ in (3.5.3) is a fourth root of unity, then $e^{\mathrm{i}2\mu_\lambda} = \pm 1$. In this case, $\mathbf{x}$ and $\overline{\mathbf{x}}$ are 2-strongly cospectral. Thus, like real pure states, non-real pure states can be 2-strongly cospectral.

We close this section with an example that illustrates Theorems 3.5.12 and 3.5.15.

Example 3.5.17. Let $A = A(K_2)$ and consider the matrices $E_1 = \frac{1}{2}J$ and $E_2 = I - \frac{1}{2}J$ in Example 3.1.3. Then:

- $E_1\mathbf{e}_1 = E_1\mathbf{e}_2$ and $E_2\mathbf{e}_1 = -E_2\mathbf{e}_2$.
- $E_1(\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2) = -\mathrm{i}E_1(\mathbf{e}_1 - \mathrm{i}\mathbf{e}_2)$ and $E_2(\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2) = \mathrm{i}E_2(\mathbf{e}_1 - \mathrm{i}\mathbf{e}_2)$.

Thus, $\{\mathbf{e}_1, \mathbf{e}_2\}$ and $\{\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2, \mathbf{e}_1 - \mathrm{i}\mathbf{e}_2\}$ are strongly cospectral pairs of pure states in K_2 to relative to A. Alternatively, if $\mathbf{u} = \mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{v} = \mathbf{e}_1 - \mathbf{e}_2$, then

$$\mathbf{e}_1 = \tfrac{1}{2}(\mathbf{u} + \mathbf{v}) \quad \text{and} \quad \mathbf{e}_1 = \tfrac{1}{2}(\mathbf{u} - \mathbf{v})$$

so that $\mathbf{e}_1$ and $\mathbf{e}_2$ are strongly cospectral by Theorem 3.5.12 with $\zeta_1 = 1$ and $\zeta_2 = -1$. Moreover, since $\mathbf{e}_1 - \mathrm{i}\mathbf{e}_2 = \overline{\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2}$ and

$$\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2 = \tfrac{e^{\mathrm{i}\pi/4}}{\sqrt{2}}\mathbf{u} + \tfrac{e^{-\mathrm{i}\pi/4}}{\sqrt{2}}\mathbf{v},$$

it follows from Theorem 3.5.15 that $\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2$ and $\mathbf{e}_1 - \mathrm{i}\mathbf{e}_2$ are strongly cospectral with $\zeta_1 = e^{\mathrm{i}2(\pi/4)} = \mathrm{i}$ and $\zeta_2 = e^{-\mathrm{i}2(\pi/4)} = -\mathrm{i}$.

3.6 Composite systems

In this section, we study quantum walks that can be viewed as a composite system of 'smaller' quantum walks. That is, quantum walks whose transition matrices can be derived from the transition matrices of smaller quantum walks comprising them. This includes quantum walks modeled by Cartesian products, direct products, joins and blow-ups of graphs. In this section, we focus on the first three, and deal with blow-up graphs later in Chapter 8.

3.6.1 Cartesian products

Let M_1 and M_2 be real symmetric matrices. It is known that

$$\operatorname{spec}(M_1 \otimes I + I \otimes M_2) = \{\lambda + \theta : \lambda \in \operatorname{spec}(M_1), \theta \in \operatorname{spec}(M_2)\}. \tag{3.6.1}$$

Since $M_1 \otimes I$ and $I \otimes M_2$ commute, we may derive the transition matrix relative to the Hamiltonian $M_1 \otimes I + I \otimes M_2$ as follows:

$$\begin{aligned} U_{M_1\otimes I + I \otimes M_2}(t) &= e^{\mathrm{i}t(M_1 \otimes I + I \otimes M_2)} \\ &= e^{\mathrm{i}t(M_1\otimes I)}e^{\mathrm{i}t(I\otimes M_2)} \\ &= (U_{M_1}(t) \otimes I)(I \otimes U_{M_2}(t)) \\ &= U_{M_1}(t) \otimes U_{M_2}(t). \end{aligned} \tag{3.6.2}$$

Consequently, the quantum walk on $M_1 \otimes I + I \otimes M_2$ can be viewed as a composite of the quantum walks with Hamiltonians M_1 and M_2.

For $j \in \{1, 2\}$, let X_j be a weighted graph on n_j vertices with adjacency matrix A_j and degree matrix D_j. The *Cartesian product* $X_1 \square X_2$ of X_1 and X_2 is the graph with vertex set $V(X_1) \times V(X_2)$ where vertices (u, x) and (v, y) are adjacent in $X_1 \square X_2$ if and only if either $u = v$ and $\{x, y\}$ is an edge in X_2 or $x = y$ and $\{u, v\}$ is an edge in X_1. The weight of the edge between (u, x) and (v, y) is equal to the weight of $\{u, v\}$ if $x = y$ and $\{x, y\}$ if $u = v$. If $u \in V(X_1)$ and $x \in V(X_2)$ have loops of weight ω and ω' in X_1 and X_2 respectively, then (u, x) also has a loop of weight $\omega + \omega'$ in $X_1 \square X_2$. The degree and adjacency matrices of $X_1 \square X_2$ are given by

$$D = (D_1 \otimes I_{n_2}) + (I_{n_1} \otimes D_2) \quad \text{and} \quad A = (A_1 \otimes I_{n_2}) + (I_{n_1} \otimes A_2)$$

respectively. In particular, if $M_1 = \alpha D_1 + A_1$ and $M_2 = \alpha D_2 + A_2$, then

$$\begin{aligned} M_1 \otimes I_{n_2} + I_{n_1} \otimes M_2 &= (\alpha D_1 + A_1) \otimes I_{n_2} + I_{n_1} \otimes (\alpha D_2 + A_2) \\ &= (\alpha(D_1 \otimes I_{n_2}) + (A_1 \otimes I_{n_2})) + (\alpha(I_{n_1} \otimes D_2) + (I_{n_1} \otimes A_2)) \\ &= \alpha[(D_1 \otimes I_{n_2}) + (I_{n_1} \otimes D_2)] + [(A_1 \otimes I_{n_2})) + (I_{n_1} \otimes A_2)] \\ &= \alpha D + A. \end{aligned}$$

In this case, the Hamiltonian $M_1 \otimes I_{n_2} + I_{n_1} \otimes M_2$ represents a generalised adjacency matrix of the Cartesian product of two graphs whose generalised adjacency matrices are given by M_1 and M_2. Making use of (3.4.2), we get

$$U_{X_1 \square X_2}(t) = U_{X_1}(t) \otimes U_{X_2}(t) \tag{3.6.3}$$

whenever the Hamiltonian taken is a generalised adjacency matrix $\alpha D + A$ for a fixed α. In other words, we may view the physical system modeled by $X_1 \square X_2$ as a composite of the physical systems modeled by X_1 and X_2 relative to $\alpha D + A$.

We denote the dth Cartesian power of X as $X^{\square d}$, which is the Cartesian product of X with itself d times. The transition matrix of $X^{\square d}$ relative to $\alpha D + A$ is

$$U_{X^{\square d}}(t) = U_X(t)^{\otimes d}, \tag{3.6.4}$$

where $U_X(t)^{\otimes d}$ is the dth tensor power of $U_X(t)$, which is simply the tensor product of $U_X(t)$ with itself d times.

Example 3.6.1. The hypercube Q_d of dimension is the graph obtained from taking the dth Cartesian power of K_2. Making use of (3.6.4) and (3.1.7), we obtain the following transition matrix for Q_d relative to A:

$$U_{Q_d}(t) = \begin{bmatrix} \cos t & \mathrm{i}\sin t \\ \mathrm{i}\sin t & \cos t \end{bmatrix}^{\otimes d}. \tag{3.6.5}$$

Note that $U_{Q_d}(\pi) = -I$, $U_{Q_d}(\frac{\pi}{2}) = (\mathrm{i})^d R_{2^d}$ where R_{2^d} is the 2^d-by-2^d reversal matrix, and $U_{Q_d}(\frac{\pi}{4})$ has all entries with magnitude equal to $\frac{1}{\sqrt{2^d}}$. In particular, we see that $U_{Q_d}(\frac{\pi}{2})\mathbf{e}_a = (\mathrm{i})^d \mathbf{e}_{2^d+1-a}$ for each vertex $a \in \{1, \dots, 2^d\}$ of Q^d.

3.6.2 Direct products

Let M_1 and M_2 be real symmetric matrices and $M_1 = \sum_{\lambda \in \operatorname{spec}(M)} \lambda E_\lambda$ be the spectral decomposition of M_1. It is known that

$$\operatorname{spec}(M_1 \otimes M_2) = \{\lambda\theta : \lambda \in \operatorname{spec}(M_1), \theta \in \operatorname{spec}(M_2)\}. \tag{3.6.6}$$

The transition matrix relative to the Hamiltonian $M_1 \otimes M_2$ is given by

$$U_{M_1 \otimes M_2}(t) = \sum_{\lambda \in \operatorname{spec}(M_1)} E_\lambda \otimes U_{M_2}(\lambda t). \tag{3.6.7}$$

For $j \in \{1, 2\}$, let X_j be weighted graphs on n_j vertices. The *direct product* $X_1 \times X_2$ of X_1 and X_2 is the graph with vertex set $V(X_1) \times V(X_2)$ where (u, x) and (v, y) are adjacent in $X_1 \times X_2$ if $\{u, v\}$ and $\{x, y\}$ are edges in X_1 and X_2, respectively. The weight of the edge between (u, x) and (v, y) is equal to the product of the weights of the edges $\{u, v\}$ and $\{x, y\}$. If $x \neq y$ and $\{x, y\}$ is an edge in Y, then (u, x) and (u, y) are adjacent in $X_1 \times X_2$ if and only if vertex u has a loop in X_1, and vertex (u, x) has a loop in $X_1 \times X_2$ if and only if vertices u and x have loops in X_1 and X_2, respectively. The adjacency matrix of $X_1 \times X_2$ is given by

$$A(X_1 \times X_2) = A(X_1) \otimes A(X_2).$$

In particular, $K_2 \times Y$ is the *bipartite double* of a weighted graph Y. Note that $K_2 \times Y$ is bipartite, and this graph is connected if and only if Y is non-bipartite.

Let $A = A(X_1 \times X_2)$. If $A(X_1) = \sum\limits_{\lambda \in \mathrm{spec}(A(X_1))} \lambda E_\lambda$ is the spectral decomposition of $A(X_1)$, then it follows from (3.6.7) that

$$U_A(t) = \sum_{\lambda \in \mathrm{spec}(A(X_1))} E_\lambda \otimes U_{A(X_2)}(\lambda t). \tag{3.6.8}$$

Thus, for the direct product $X_1 \times X_2$, the transition matrix $U_A(t)$ can be derived from $U_{A(X_2)}(t)$ and the spectral information of $A(X_1)$.

3.6.3 Joins

For $j \in \{1, 2\}$, let X_j be simple weighted graphs on n_j vertices. The *join* of X_1 and X_2, denoted $X_1 \vee X_2$, is a graph on $n = n_1 + n_2$ vertices obtained from taking a copy of X_1, a copy of X_2 and inserting all edges between X_1 and X_2 with weight one. Equivalently,

$$A(X_1 \vee X_2) = \begin{bmatrix} A(X_1) & J \\ J & A(X_1) \end{bmatrix}.$$

The graph $O_1 \vee Y$ is a *cone* on Y and the lone vertex in O_1 is called an *apex* of the cone. Meanwhile, if $X \in \{O_2, K_2\}$, then $X \vee Y$ is called a *double cone* on Y, and the vertices of $X \in \{O_2, K_2\}$ are the *apices* of the double cone. In particular, $O_2 \vee Y$ and $K_2 \vee Y$ are called the *disconnected* and *connected* double cones on Y, respectively.

In this subsection, we focus on the case $M \in \{A, L\}$ with the additional assumption that X_1 and X_2 are weighted k- and ℓ-regular graphs, resp., when $M = A$.

Let $L = L(X_1 \vee X_2)$. If X_1 and X_2 are connected, then it is known that

$$\mathrm{spec}(L) = \{0, n\} \cup \{\lambda + n_2 : \lambda \in \mathrm{spec}(L(X_1)) \backslash \{0\}\} \cup \{\mu + n_1 : \mu \in \mathrm{spec}(L(X_2)) \backslash \{0\}\}. \tag{3.6.9}$$

while if X_1 (resp., X_2) is disconnected then we simply include n_2 (resp., n_1) in $\mathrm{spec}(L)$. In particular, 0 is a simple eigenvalue of L with eigenvector $\mathbf{1}$ and n is an eigenvalue of L with associated eigenvector $\begin{bmatrix} n_2 \mathbf{1}_{n_1} \\ -n_1 \mathbf{1}_{n_2} \end{bmatrix}$. Moreover, if $\mathbf{u}$ and $\mathbf{v}$ are eigenvectors associated with $\lambda > 0$ and $\mu > 0$ for $L(X_1)$ and $L(X_2)$, then $\begin{bmatrix} \mathbf{u} \\ \mathbf{0} \end{bmatrix}$ and $\begin{bmatrix} \mathbf{0} \\ \mathbf{v} \end{bmatrix}$ are eigenvectors associated with $\lambda + n_2$ and $\mu + n_1$ respectively. From [1, Equation 33], we obtain the transition matrix of $X_1 \vee X_2$ relative to the Hamiltonian L when X_1 and X_2 are connected:

$$U_L(t) = \frac{1}{n}J + e^{\mathrm{i}tn}E_n + \sum_{\lambda>0} e^{\mathrm{i}t(\lambda+n_2)} \begin{bmatrix} E_\lambda & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} + \sum_{\mu>0} e^{\mathrm{i}t(\mu+n_1)} \begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & F_\mu \end{bmatrix}, \tag{3.6.10}$$

where $E_n = \frac{1}{n_1n_2n}\begin{bmatrix} n_2^2J & -n_1n_2J \\ -n_1n_2J & n_1^2J \end{bmatrix}$ and F_μ is the spectral idempotent of $\mu \in \operatorname{spec}(L(X_2))\backslash\{0\}$. We include $e^{\mathrm{i}tn_2}\begin{bmatrix} E_0 - \frac{1}{n_1}J & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$ (resp., $e^{\mathrm{i}tn_1}\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & F_0 - \frac{1}{n_2}J \end{bmatrix}$) as a term in the third (resp., fourth) summand in (3.6.10) when X_1 (resp., X_2) is disconnected. Using the spectral decompositions of $U_{L(X_1)}(t)$ and $U_{L(X_2)}(t)$, we may write (3.6.10) as

$$U_L(t) = \frac{1}{n}J + e^{\mathrm{i}tn}E_n + \begin{bmatrix} e^{\mathrm{i}tn_2}(U_{L(X_1)}(t) - \frac{1}{n_1}J) & \mathbf{0} \\ \mathbf{0} & e^{\mathrm{i}tn_1}(U_{L(X_2)}(t) - \frac{1}{n_2}J) \end{bmatrix}. \tag{3.6.11}$$

Now, let $A = A(X_1 \vee X_2)$ and suppose further that X_1 and X_2 are weighted k- and ℓ-regular graphs, respectively. Let

$$\lambda^{\pm} = \frac{1}{2}(k + \ell \pm \sqrt{\Delta}), \quad \text{where } \Delta = (k-\ell)^2 + 4n_1n_2. \tag{3.6.12}$$

If X_1 and X_2 are connected, then it is known that

$$\operatorname{spec}(A) = \{\lambda^{\pm}\} \ \cup \ \operatorname{spec}(A(X_1))\backslash\{k\} \ \cup \ \operatorname{spec}(A(X_2))\backslash\{\ell\}. \tag{3.6.13}$$

while if X_1 (resp., X_2) is disconnected then we simply include k (resp., ℓ) in $\operatorname{spec}(L)$. Now, set

$$E_{\lambda^+} = \frac{1}{n_1\sqrt{\Delta}(k-\lambda^-)}\mathbf{u}\mathbf{u}^T \quad \text{and} \quad E_{\lambda^-} = \frac{1}{n_1\sqrt{\Delta}(\lambda^+-k)}\mathbf{v}\mathbf{v}^T,$$

where $\mathbf{u} = \begin{bmatrix} (k-\lambda^-)\mathbf{1}_{n_1} \\ n_1\mathbf{1}_{n_2} \end{bmatrix}$ and $\mathbf{v} = \begin{bmatrix} (k-\lambda^+)\mathbf{1}_{n_1} \\ n_1\mathbf{1}_{n_2} \end{bmatrix}$ are eigenvectors associated with λ^+ and λ^-, respectively. Moreover, if $\mathbf{w}$ and $\mathbf{z}$ are eigenvectors associated with $\lambda \in \operatorname{spec}(A(X_1))\backslash\{k\}$ and $\mu \in \operatorname{spec}(A(X_2))\backslash\{\ell\}$, then $\begin{bmatrix} \mathbf{w} \\ \mathbf{0} \end{bmatrix}$ and $\begin{bmatrix} \mathbf{0} \\ \mathbf{z} \end{bmatrix}$ are eigenvectors associated with λ and θ for $A(X \vee Y)$ respectively. From [37, Equation 12.2.1], we obtain the transition matrix of $X_1 \vee X_2$ relative to the Hamiltonian A

when X_1 and X_2 are connected:

$$U_A(t) = e^{\mathrm{i}t\lambda^+}E_{\lambda^+} + e^{\mathrm{i}t\lambda^-}E_{\lambda^-} + \sum_{\lambda<k} e^{\mathrm{i}t\lambda}\begin{bmatrix} E_\lambda & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} + \sum_{\mu<\ell} e^{\mathrm{i}t\mu}\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & F_\mu \end{bmatrix}. \tag{3.6.14}$$

We include the term $e^{\mathrm{i}tk}\begin{bmatrix} E_0 - \frac{1}{n_1}J & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix}$ (resp., $e^{\mathrm{i}t\ell}\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & F_0 - \frac{1}{n_2}J \end{bmatrix}$) in the third (resp., fourth) summand in equation (3.6.14) whenever X_1 (resp., X_2) is disconnected. Using the spectral decompositions of $U_{A(X_1)}(t)$ and $U_{A(X_2)}(t)$ and the fact that X_1 and X_2 are weighted-regular, we may write (3.6.10) as

$$U_A(t) = e^{\mathrm{i}t\lambda^+}E_{\lambda^+} + e^{\mathrm{i}t\lambda^-}E_{\lambda^-} + \begin{bmatrix} U_{A(X_1)}(t) - \frac{1}{n_1}J & \mathbf{0} \\ \mathbf{0} & U_{A(X_2)}(t) - \frac{1}{n_2}J) \end{bmatrix}. \tag{3.6.15}$$

From (3.6.11) (resp., (3.6.15)), it follows that we can express the transition matrix $U_L(t)$ (resp., $U_A(t)$) of $X_1 \vee X_2$ in terms of the transition matrices $U_{L(X_1)}(t)$ and $U_{L(X_2)}(t)$ (resp., $U_{A(X_1)}(t)$ and $U_{A(X_2)}(t)$) of X_1 and X_2, respectively.

3.7 Periodicity

In this section, we define and characterise periodicity of complex vectors and quantum walks, and compute a related parameter called the minimum period.

Definition 3.7.1. Suppose $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ is not a fixed state. We say that $\mathbf{x}$ is *periodic* (in X relative to M) if there is a time $\tau > 0$ and a complex number γ such that

$$U(\tau)\mathbf{x} = \gamma\mathbf{x}. \tag{3.7.1}$$

The minimum such $\tau > 0$ is called the *minimum period* of $\mathbf{x}$, which we denote by ρ.

Example 3.7.2. From Example 3.1.3, one checks that $U(\pi)\mathbf{e}_j = -\mathbf{e}_j$ for $j \in \{1, 2\}$. That is, $\mathbf{e}_1$ and $\mathbf{e}_2$ are periodic in K_2 relative to A at time π.

We now characterise periodicity of complex vectors. Suppose $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ is not a fixed state, so that $|\Phi_{\mathbf{x}}| \geq 2$. Suppose the spectral decomposition of M is given by

$$M = \sum_{\lambda \in \operatorname{spec}(M)} \lambda E_\lambda.$$

From the definition, $\mathbf{x}$ is periodic if and only if $U(\tau)\mathbf{x} = \gamma\mathbf{x}$. Using the spectral decomposition of M, we may write this equation as

$$\sum_{\lambda \in \Phi_{\mathbf{x}}} e^{\mathrm{i}\tau\lambda} E_\lambda \mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}}} \gamma E_\lambda \mathbf{x}.$$

Since the E_λ's are pairwise multiplicatively orthogonal, we obtain

$$e^{\mathrm{i}\tau\lambda} = \gamma \quad \text{for each } \lambda \in \Phi_{\mathbf{x}}. \tag{3.7.2}$$

Equivalently, for all $\lambda, \theta \in \Phi_{\mathbf{x}}$, there exists an integer $k_{\lambda,\theta}$ such that

$$\tau(\lambda - \theta) = 2k_{\lambda,\theta}\pi. \tag{3.7.3}$$

That is, (2.3.3) holds for all $\lambda, \theta, \alpha, \beta \in \Phi_{\mathbf{x}}$ with $\alpha \neq \beta$. From this observation, the following result is immediate.

Theorem 3.7.3. *Suppose* $\mathbf{x} \in \mathbb{C}^n \backslash \{\mathbf{0}\}$ *is not a fixed state. Then* $\mathbf{x}$ *is periodic if and only if* $\Phi_{\mathbf{x}}$ *satisfies the ratio condition.*

The above theorem was first established by Godsil for periodic real states [52].

Definition 3.7.4. A quantum walk (in X with Hamiltonian M) is *periodic* if every pure state $\mathbf{x} \in \mathbb{C}^n$ that is not fixed is periodic relative to M at the same time $\tau > 0$. The minimum such $\tau > 0$ is called the *minimum period*.

Theorem 3.7.5. *A quantum walk is periodic if and only if there is a time* τ *and a unit complex number* γ *such that*

$$U(\tau) = \gamma I.$$

Proof. Suppose the quantum walk on M is periodic. Since M is irreducible, every pure state of the form $\mathbf{e}_u$ is no eigenvector for M, and so by Proposition 3.3.3, such a pure state is not fixed. By definition of a periodic quantum walk, every pure state of the form $\mathbf{e}_u$ is periodic at time τ. Now, suppose $V(X) = \{1, \dots, n\}$. Making use of (3.7.2), we get that for each vertex j of X, we have

$$U(\tau)\mathbf{e}_j = e^{\mathrm{i}\tau\lambda}\mathbf{e}_j \tag{3.7.4}$$

for all $\lambda \in \Phi_{\mathbf{e}_j}$. Now, let $\gamma = e^{\mathrm{i}\tau\lambda}$ for some $\lambda \in \Phi_{\mathbf{e}_1}$. Applying Lemma 3.3.6 with $S = \{1\}$, we get that there is another index $j \in V(X)\backslash\{1\}$, say $j = 2$, such that $\Phi_{\mathbf{e}_1} \cap \Phi_{\mathbf{e}_2} \neq \varnothing$. Combining this with (3.7.4) yields

$$\gamma = e^{\mathrm{i}\tau\lambda} \quad \text{for all} \quad \lambda \in \Phi_{\mathbf{e}_1} \cup \Phi_{\mathbf{e}_2}. \tag{3.7.5}$$

Again applying Lemma 3.3.6 with $S = \{1, 2\}$, we get another index $j \in V(X)\backslash\{1, 2\}$, say $j = 3$, such that $(\Phi_{\mathbf{e}_1} \cup \Phi_{\mathbf{e}_2}) \cap \Phi_{\mathbf{e}_3} \neq \varnothing$. Combining this again with (3.7.4) and (3.7.5) yields $\gamma = e^{\mathrm{i}\tau\lambda}$ for all $\lambda \in \bigcup_{j=1}^{3} \Phi_{\mathbf{e}_j}$. Repeating this argument $n-3$ times and using the fact that $\operatorname{spec}(M) = \bigcup_{j=1}^{n} \Phi_{\mathbf{e}_j}$ yields

$$\gamma = e^{\mathrm{i}\tau\lambda} \quad \text{for all} \quad \lambda \in \operatorname{spec}(M).$$

Invoking (3.7.4) one last time, we conclude that there is a unit complex number γ such that $U(\tau)\mathbf{e}_j = \gamma\mathbf{e}_j$ for each vertex j of X. Equivalently, $(U(\tau) - \gamma I)\mathbf{e}_j = \mathbf{0}$ for each vertex j of X. This implies that all columns of $U(\tau) - \gamma I$ are zero, and so it must be that $U(\tau) = \gamma I$. Conversely, if $U(\tau) = \gamma I$, then $U(\tau)\mathbf{x} = \gamma\mathbf{x}$ for each $\mathbf{x} \in \mathbb{C}^n$ that is not fixed. That is, the quantum walk on M is periodic. □

Remark 3.7.6. If a quantum walk is periodic with minimum period ρ and phase factor γ, then for all integers q, it is also periodic at time $q\rho$ with factor γ^q since

$$U(q\tau) = U(\tau)^q = (\gamma I)^q = \gamma^q I,$$

where the second equation above follows from Theorem 3.7.5. Similarly, if $\mathbf{x}$ is periodic with period τ and phase factor γ, then $\mathbf{x}$ is also periodic at time $q\tau$ with factor γ^q.

Theorem 3.7.7. *A quantum walk is periodic if and only if* $\operatorname{spec}(M)$ *satisfies the ratio condition.*

Proof. Suppose the quantum walk on M is periodic. Equivalently, $U(\tau) = \gamma I$ for some time $\tau > 0$ by Theorem 3.7.5. If $M = \sum_{\lambda\in\operatorname{spec}(M)} \lambda E_\lambda$ is the spectral decomposition of M, then it follows that

$$U(\tau) \;=\; \sum_{\lambda\in\operatorname{spec}(M)} e^{\mathrm{i}\tau\lambda} E_\lambda \;=\; \gamma I.$$

Since the E_λ's sum to the identity, the above equation holds if and only if $e^{\mathrm{i}\tau\lambda} = \gamma$ for all $\lambda \in \operatorname{spec}(M)$. Replacing $\Phi_{\mathbf{x}}$ by $\operatorname{spec}(M)$ in (3.7.2), the preceding condition is equivalent to $\operatorname{spec}(M)$ satisfying the ratio condition. □

The following result calculates the minimum period of any periodic complex vector. It was first established by Kirkland, Monterde and Plosker for periodic vertex states [67, Theorem 5], but it applies to any complex vector.

Theorem 3.7.8. *Let* $\mathbf{x} \in \mathbb{C}^n$ *with* $\Phi_{\mathbf{x}} = \{\lambda_1, \ldots, \lambda_r\}$. *The following hold.*

1. *If* $r = 2$, *then* $\mathbf{x}$ *is periodic with* $\rho = \frac{2\pi}{|\lambda_1 - \lambda_2|}$

2. *If* $r \geq 3$ *and* $\mathbf{x}$ *is periodic, then* $\rho = \frac{2\pi q}{|\lambda_1 - \lambda_2|}$, *where* $q = \operatorname{lcm}(q_3, \dots, q_r)$ *and the* p_j*'s and* q_j*'s are integers satisfying* $\frac{\lambda_1 - \lambda_j}{\lambda_1 - \lambda_2} = \frac{p_j}{q_j}$ *and* $\gcd(p_j, q_j) = 1$.

In both cases, every period τ *of* $\mathbf{x}$ *is an integer multiple of* ρ.

Proof. First, suppose $r = 2$. By (3.7.3), $\mathbf{x}$ is periodic at time τ if and only if $\tau(|\lambda_1 - \lambda_2|) = 2k\pi$ for some integer k. This proves that $\mathbf{x}$ is periodic with $\rho = \frac{2\pi}{|\lambda_1 - \lambda_2|}$. To prove 2, suppose $m \geq 3$ and $\mathbf{x}$ is periodic. Theorem 3.7.3 allows us to write $\frac{\lambda_1 - \lambda_j}{\lambda_1 - \lambda_2} = \frac{p_j}{q_j}$, where p_j's and q_j's are integers satisfying $\gcd(p_j, q_j) = 1$. Now, assume that $\rho = \frac{2\pi z}{|\lambda_1 - \lambda_2|}$ for some $z \in \mathbb{R}$. Since $\gcd(p_j, q_j) = 1$ for each $j \geq 2$, we get that $\rho(\lambda_1 - \lambda_j) = 2\pi z \left(\frac{\lambda_1 - \lambda_j}{|\lambda_1 - \lambda_2|}\right) = \pm \frac{2\pi z p_j}{q_j}$ is an integer multiple of 2π if and only if z is the minimum integer such that each q_j divides z. Therefore, $z = q$, where $q = \operatorname{lcm}(q_2, \dots, q_r)$ and so $\rho = \frac{2\pi q}{|\lambda_1 - \lambda_2|}$. Moreover, it is clear from (3.7.3) that every period τ is an integer multiple of ρ. □

Remark 3.7.9. From (3.7.3), the ρ in Theorem 3.7.8 is the least $\tau > 0$ such that $\tau(\lambda - \theta)$ is an integer multiple of 2π for all $\lambda, \theta \in \Phi_{\mathbf{x}}$.

Combining Theorem 2.3.5 with Theorems 3.7.3 and 3.7.8 yields the following number-theoretic characterisation of periodicity.

Theorem 3.7.10. *Let* $\mathbf{x} \in \mathbb{C}^n$ *with* $|\Phi_{\mathbf{x}}| \geq 3$, *and* $\Phi_{\mathbf{x}}$ *be a set of real algebraic numbers closed under taking algebraic conjugates. Then* $\mathbf{x}$ *is periodic if and only if either of the following holds.*

1. *All elements in* $\Phi_{\mathbf{x}}$ *are rationals.*

2. *All elements in* $\Phi_{\mathbf{x}}$, *except possibly one, are quadratic irrationals, and there is a square-free integer* $\Delta > 1$ *and* $a, b_j \in \mathbb{Q}$ *such that each* $\lambda_j \in \Phi_{\mathbf{x}}$ *can be written as* $\lambda_j = \frac{1}{2}(a + b_j\sqrt{\Delta})$. *Moreover, exactly one element* θ *in* $\Phi_{\mathbf{x}}$ *is rational if and only if* $|\Phi_{\mathbf{x}}|$ *is odd, in which case* $\theta = \frac{a}{2}$.

Additionally, if $\Phi_{\mathbf{x}}$ *is a set of real algebraic integers, then we may replace the terms 'rationals' and 'irrationals' by 'integers' in conditions 1 and 2 and we may express*

$$\rho = \frac{2\pi}{g\sqrt{\Delta}} \tag{3.7.6}$$

where $g = \gcd\{\frac{\lambda_1 - \lambda_2}{\sqrt{\Delta}}, \dots, \frac{\lambda_1 - \lambda_r}{\sqrt{\Delta}}\}$ *and* $\Delta = 1$ *whenever condition 1 holds.*

Proof. Theorems 2.3.5 and 3.7.3 yield the above equivalence. Since $\Phi_{\mathbf{x}}$ is closed under algebraic conjugates, exactly one eigenvalue $\Phi_{\mathbf{x}}$ is rational if and only if $|\Phi_{\mathbf{x}}|$ is odd. Now, suppose $\theta \in \Phi_{\mathbf{x}}$ be rational. If $\lambda \in \Phi_{\mathbf{x}} \backslash \{\theta\}$ is a quadratic irrational of the form $\lambda = \frac{1}{2}(a + b_j\sqrt{\Delta})$, then by assumption, its conjugate $\mu = \frac{1}{2}(a - b_j\sqrt{\Delta})$ also belongs to $\Phi_{\mathbf{x}} \backslash \{k\}$. From Theorem 3.7.3, $\Phi_{\mathbf{x}}$ is periodic if and only if

$$\frac{\theta - \lambda}{\theta - \mu} = \frac{2\theta - a - b_j\sqrt{\Delta}}{2\theta - a + b_j\sqrt{\Delta}} \in \mathbb{Q}$$

for all $\lambda, \mu \in \Phi_{\mathbf{x}} \backslash \{k\}$. Since $\sqrt{\Delta} \notin \mathbb{Q}$, the above equation holds if and only if $a = 2\theta$. Finally, we prove (3.7.6). Suppose $\Phi_{\mathbf{x}}$ is a set of real algebraic integers so that we can write each λ_j as $\lambda_j = \frac{1}{2}(a + b_j\sqrt{\Delta})$, where $\Delta \geq 1$ and a, b_j are integers. Then we may write each q_j in Theorem 3.7.8(2) as $q_j = \frac{b_1 - b_2}{2g_j}$, where $g_j = \gcd(b_1 - b_j, b_1 - b_2)$. Thus, $q = \operatorname{lcm}(q_j) = \operatorname{lcm}\left(\frac{b_1-b_2}{2g_3}, \ldots, \frac{b_1-b_2}{2g_m}\right) = \frac{b_1-b_2}{g} = \frac{\lambda_1-\lambda_2}{g\sqrt{\Delta}}$. Thus $\rho = \frac{2\pi q}{\lambda_1 - \lambda_2} = \frac{2\pi}{g\sqrt{\Delta}}$. □

Remark 3.7.11. In Theorem 3.7.10(2), at most one eigenvalue in $\Phi_{\mathbf{x}}$ is rational.

In Theorem 3.7.10, the case when $\Phi_{\mathbf{x}}$ is a set of real algebraic integers was first observed by Godsil [48, Corollary 3.3], and later established by Coutinho and Godsil [37, Corollary 7.6.2]. The more general case when $\Phi_{\mathbf{x}}$ is a set of real algebraic numbers was shown by Coutinho and Baptista [34, Lemma 3.2].

Combining Theorem 3.7.10 with Theorems 3.7.3 and 3.7.7 yields an analogous result for periodicity of quantum walks.

Theorem 3.7.12. *Suppose* $\operatorname{spec}(M)$ *is a set of real algebraic numbers, closed under taking algebraic conjugates. The quantum walk on M is periodic if and only if either of the two conditions in Theorem 3.7.10 holds whenever $\Phi_{\mathbf{x}}$ is replaced by* $\operatorname{spec}(M)$.

Corollary 3.7.13. *The following hold.*

1. *Let $\Phi_{\mathbf{x}}$ be a set of real algebraic integers closed under taking algebraic conjugates and let $\theta \in \Phi_{\mathbf{x}}$ be an integer. Then $\mathbf{x}$ is periodic if and only if either $\Phi_{\mathbf{x}} \subseteq \mathbb{Z}$, or each $\lambda_j \in \Phi_{\mathbf{x}}$ is a quadratic integer of the form $\lambda_j = \theta + b_j\sqrt{\Delta}$ for some square-free integer $\Delta > 1$ and nonzero integers $b_1, \ldots, b_r$. If the latter condition holds, then $|\Phi_{\mathbf{x}}|$ is odd. This statement holds if we replace $\Phi_{\mathbf{x}}$ by* $\operatorname{spec}(M)$.

2. *Let* $\operatorname{spec}(M)$ *be a set of real algebraic integers closed under algebraic conjugates. If the trace of M equals 0, then the quantum walk on M is periodic if and only if either* $\operatorname{spec}(M) \subseteq \mathbb{Z}$, *or all elements of* $\operatorname{spec}(M)$ *are integer multiples of $\sqrt{\Delta}$ for some square-free integer $\Delta > 1$. Moreover, the latter condition holds for $M = A$ if and only if X is bipartite.*

Proof. Our assumption in 1 implies that $\Phi_{\mathbf{x}}$ is a set of real algebraic integers. Thus, we may replace the terms 'rationals' by 'integers' in Theorem 3.7.10(2). In this case, exactly one eigenvalue in $\Phi_{\mathbf{x}}$ is an integer if and only if $|\Phi_{\mathbf{x}}|$ is odd, in which case $\theta = \frac{a}{2}$. The last statement in 1 is immediate from Theorem 3.7.12. To prove 2, let the trace of M be 0. The quantum walk on M is periodic if and only if Theorem 3.7.12 holds. If all eigenvalues in spec(M) are of the form $\lambda_j = \frac{1}{2}(a + b_j\sqrt{\Delta})$, and c_j as the algebraic multiplicity of λ_j, then the trace of M being 0 is equivalent to

$$0 = \sum_{\lambda_j \in \operatorname{spec}(M)} c_j\lambda_j = \sum_{\lambda_j \in \operatorname{spec}(M)} (c_j/2)(a + b_j\sqrt{\Delta}) = a|V(X)|/2 + \sqrt{\Delta} \sum_{\lambda_j \in \operatorname{spec}(M)} b_j.$$

Since $a|V(X)|/2 \in \mathbb{Q}$ and $\sqrt{\Delta} \notin \mathbb{Q}$, the above equation gives us $\sum_{\lambda_j \in \operatorname{spec}(M)} b_j = 0$ and $a = 0$. Thus, spec$(M) \subseteq \mathbb{Z}$, or all elements of spec(M) are integer multiples of $\sqrt{\Delta}$ for some square-free integer $\Delta > 1$. If $M = A$, then the latter condition implies that spec(A) is closed under multiplication by -1. Equivalently, X is bipartite. $\square$

The last statement in Corollary 3.7.13(2) is due to Godsil [48, Corollary 3.3].

Example 3.7.14. For P_3, spec$(A) = \{0, \pm\sqrt{2}\}$. Thus, for $P_3^{\square n}$, all elements of spec(A) are integer multiples of $\sqrt{2}$ by (3.6.1). Invoking Corollary 3.7.13(2), we get that $P_3^{\square n}$ is periodic relative to A. We also note that $P_3^{\square n}$ is bipartite for all $n \geq 1$.

A weighted *walk-regular graph* X is a weighted-regular graph such that every pair of vertices are cospectral. Some well-known families of unweighted walk-regular graphs include distance-regular graphs, vertex-transitive graphs, graphs in coherent configurations (including association schemes). As the trace of each E_λ is equal to the multiplicity c_λ of λ as an eigenvalue of A divided by $|V(X)|$, a weighted walk-regular graph satisfies $(E_\lambda)_{u,u} = \frac{c_\lambda}{|V(X)|} \neq 0$ for each $\lambda \in \operatorname{spec}(A)$. Since $E_\lambda \mathbf{e}_u = \mathbf{0}$ if and only if $(E_\lambda)_{u,u} = 0$, we get the following result.

Proposition 3.7.15. *If X is weighted walk-regular, then $\Phi_{\mathbf{e}_u}(X) = \operatorname{spec}(A(X))$.*

For more about walk-regular graphs, we refer the reader to [37, Section 6.3].

From Proposition 3.7.15, if X is weighted walk-regular, then any statement pertaining to $\Phi_{\mathbf{e}_u}(X)$ applies to spec$(A(X))$ and vice versa.

Corollary 3.7.16. *Suppose X is a weighted walk-regular with valency d and $\phi(A, t)$ has integer coefficients. The following are equivalent.*

1. *All eigenvalues of A are integers.*

2. *Each vertex of X is periodic relative to A.*

3. *The quantum walk on X is periodic relative to A.*

Proof. By assumption, the largest eigenvalue d of A is an integer. Corollary 3.7.13(2) and Proposition 3.7.15 yield the equivalence of 1 and 2, and 2 and 3, respectively. ☐

Since X is regular in Proposition 3.7.15 and Corollary 3.7.16, these results also apply to $\alpha D + A$ for all $\alpha \in \mathbb{R}$.

The next result is immediate from Corollary 3.7.13(1) and the facts that L is positive semidefinite and $0 \in \Phi_{\mathbf{e}_u}$ for each vertex u of X.

Theorem 3.7.17. *If $\phi(L(X), t)$ has integer coefficients, then u in X is Laplacian periodic if and only if $\Phi_{\mathbf{e}_u}(X) \subset \mathbb{Z}$. In this case, $\rho_u = \frac{2\pi}{g}$, where $g = \gcd(\Phi_{\mathbf{e}_u}(X) \backslash \{0\})$.*

The following result is derived from Theorem 3.7.10. It may be viewed as an extension of [53, Corollary 9] and [64, Corollary 3.4].

Corollary 3.7.18. *Let $\mathbf{x} \in \mathbb{C}^n$ with $|\Phi_{\mathbf{x}}| \geq 3$. If $\Phi_{\mathbf{x}}$ (respectively, $\operatorname{spec}(M)$) is a set of real algebraic integers, closed under taking algebraic conjugates and $\mathbf{x}$ (respectively, M) is periodic, then $|\lambda - \theta| \geq 1$ for all $\lambda, \theta \in \Phi_{\mathbf{x}}$ (respectively, $\lambda, \theta \in \operatorname{spec}(M)$).*

We close this section with some results about constructing periodic pure states and quantum walks. The first one immediate from (3.6.2).

Theorem 3.7.19. *The complex vector $\mathbf{x}_1 \otimes \mathbf{x}_2$ is periodic relative to $M_1 \otimes I_{n_2} + I_{n_1} \otimes M_2$ at time τ if and only if $\mathbf{x}_j$ is periodic relative to M_j at time τ for $j \in \{1, 2\}$.*

We end this chapter with the following result.

Theorem 3.7.20. *Suppose the eigenvalues of M_1 and M_2 are rational. Then the quantum walks relative to M_1, M_2, $M_1 \otimes M_2$, and $M_1 \otimes I_{n_2} + I_{n_1} \otimes M_2$ are all periodic. Additionally:*

1. *If $M_1 = L(X)$ and $M_2 = L(Y)$, then the quantum walk on $L(X \vee Y)$ is also periodic.*

2. *If $M_1 = A(X)$ and $M_2 = A(Y)$ and Δ in (3.6.12) is rational, then the quantum walk on $A(X \vee Y)$ is also periodic.*

Proof. If M_1 and M_2 have rational eigenvalues, then so do $M_1 \otimes I_{n_2} + I_{n_1} \otimes M_2$ and $M_1 \otimes M_2$ from (3.6.1) and (3.6.6). If $M_1 = L(X)$ and $M_2 = L(Y)$, then from (3.6.9), $L(X \vee Y)$ has rational eigenvalues. Meanwhile, if $M_1 = A(X)$ and $M_2 = A(Y)$, then $A(X \vee Y)$ has rational eigenvalues whenever Δ in (3.6.12) is rational. Combining these facts with Theorem 3.7.3 yields the desired result. ☐

4

Perfect state transfer

From the previous chapter, we learned that if the initial state of our quantum walk on X relative to M is represented by a density matrix D, then the state $D(t)$ at time t in X relative to M is given by

$$D(t) = U_M(t) D U_M(-t).$$

We say that *perfect state transfer* (PST) occurs from a density matrix D_1 to another density matrix D_2 in X relative to M if for some time $\tau > 0$, we have

$$D_2 = U_M(\tau) D_1 U_M(-\tau).$$

Definition 4.0.1. Suppose $\mathbf{x}, \mathbf{y}$ in $\mathbb{C}^n$ are linearly independent vectors. There is *perfect state transfer* (PST) from $\mathbf{x}$ to $\mathbf{y}$ (in X relative to M) if there is a time $\tau > 0$ and a complex number γ called *phase factor* such that

$$U_M(\tau)\mathbf{x} = \gamma \mathbf{y}. \tag{4.0.1}$$

The minimum such $\tau > 0$ is called the *minimum PST time.*

Remark 4.0.2. Since $U_M(t)$ is a unitary matrix for all $t \in \mathbb{R}$ and the Euclidean norm is unitarily invariant, it follows that the complex number γ in equations (3.7.1) and (4.0.1), and the vectors $\mathbf{x}, \mathbf{y}$ in equation (4.0.1) satisfy $|\gamma| = 1$ and $\|\mathbf{x}\| = \|\mathbf{y}\|$.

If $\mathbf{x}$ and $\mathbf{y}$ in (4.0.1) are linearly dependent, then $\mathbf{x}$ is periodic. Moreover, since the equation $D_{\mathbf{y}} = U_M(\tau) D_{\mathbf{x}} U_M(-\tau)$ is equivalent to (4.0.1), the existence of perfect state transfer between density matrices $D_{\mathbf{x}}$ and $D_{\mathbf{y}}$ is equivalent to either perfect state transfer from $\mathbf{x}$ to $\mathbf{y}$ whenever they are linearly independent, or periodicity of $\mathbf{x}$ whenever $\mathbf{x}$ and $\mathbf{y}$ are linearly dependent.

Example 4.0.3. From Example 3.1.3, one checks that the following equations hold:

$$U\left(\tfrac{\pi}{2}\right)\mathbf{e}_1 = \mathrm{i}\mathbf{e}_2, \quad U\left(\tfrac{\pi}{2}\right)(\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2) = \mathbf{e}_1 - \mathrm{i}\mathbf{e}_2 \quad \text{and} \quad U\left(\tfrac{\pi}{4}\right)\mathbf{e}_1 = \tfrac{\sqrt{2}}{2}(\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2).$$

That is, perfect state transfer occurs in K_2 relative to A from the vertex state $\mathbf{e}_1$ to the vertex state $\mathbf{e}_2$ at time $\frac{\pi}{2}$, from the (i)-pair state $\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2$ to the ($-$i)-pair state $\mathbf{e}_2 - \mathrm{i}\mathbf{e}_2$ at time $\frac{\pi}{2}$, and from the vertex state $\mathbf{e}_1$ to the (i)-pair state $\mathbf{e}_1 + \mathrm{i}\mathbf{e}_2$ at $\frac{\pi}{4}$.

Our main goal in this chapter is to develop the theory of perfect state transfer on pure states in continuous quantum walks. We establish fundamental properties, provide spectral characterisations, and present constructions of pure states with PST. By virtue of Remark 4.0.2 and the definition of PST, we assume in this chapter that $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ are linearly independent vectors satisfying $\|\mathbf{x}\| = \|\mathbf{y}\| \neq \mathbf{0}$.

4.1 Characterisations

In this section, we provide the most general characterisations for PST in quantum walks.

Lemma 4.1.1. *Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ *if and only if*

$$|\mathbf{y}^* U(\tau)\mathbf{x}| = \|\mathbf{x}\|^2.$$

Equivalently, the fidelity of quantum state transfer from $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ *equals 1.*

Proof. If PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ, then $U(\tau)\mathbf{x} = \gamma\mathbf{y}$ for some unit complex number γ. Thus, $|\mathbf{y}^* U(\tau)\mathbf{x}| = |\gamma\mathbf{y}^*\mathbf{y}| = \|\mathbf{y}\|^2 = \|\mathbf{x}\|^2$. Conversely, suppose $|\mathbf{y}^* U(\tau)\mathbf{x}| = \|\mathbf{x}\|^2$. Let $\overline{\gamma} = \frac{|\mathbf{y}^* U(\tau)^*\mathbf{x}|}{\mathbf{y}^* U(\tau)^*\mathbf{x}}$, which is a unit complex number. Then

$$\begin{aligned}
\|U(\tau)\mathbf{x} - \gamma\mathbf{y}\|^2 &= (U(\tau)\mathbf{x} - \gamma\mathbf{y})^*(U(\tau)\mathbf{x} - \gamma\mathbf{y}) \\
&= \mathbf{x}^*\mathbf{x} + \mathbf{y}^*\mathbf{y} - (\gamma\mathbf{x}^* U(\tau)^*\mathbf{y} + \overline{\gamma}\mathbf{y}^* U(\tau)\mathbf{x}) \\
&= 2\|\mathbf{x}\|^2 - 2\operatorname{Re}(\overline{\gamma}\mathbf{y}^* U(\tau)\mathbf{x}) \\
&= 2\|\mathbf{x}\|^2 - 2\operatorname{Re}(|\mathbf{y}^* U(\tau)\mathbf{x}|) \\
&= 2(\|\mathbf{x}\|^2 - |\mathbf{y}^* U(\tau)\mathbf{x}|) \\
&= 0.
\end{aligned}$$

Equivalently, PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ. □

The next lemma is an extension of the three inequalities in Section 7.1 [37].

Lemma 4.1.2. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. *For any time* t, *the following inequalities hold.*

$$\begin{aligned}
\frac{1}{\|\mathbf{x}\|^2}|\mathbf{y}^* U(t)\mathbf{x}| &\leq \frac{1}{\|\mathbf{x}\|^2} \sum_{\lambda \in \Phi_{\mathbf{x}}} |(E_\lambda \mathbf{y})^*(E_\lambda \mathbf{x})| && (4.1.1)\\
&\leq \frac{1}{\|\mathbf{x}\|^2} \sum_{\lambda \in \Phi_{\mathbf{x}}} \|E_\lambda \mathbf{y}\| \cdot \|E_\lambda \mathbf{x}\| && (4.1.2)\\
&\leq \frac{1}{\|\mathbf{x}\|^2} \sqrt{\sum_{\lambda \in \Phi_{\mathbf{x}}} \|E_\lambda \mathbf{y}\|^2} \cdot \sqrt{\sum_{\lambda \in \Phi_{\mathbf{x}}} \|E_\lambda \mathbf{x}\|^2} && (4.1.3)\\
&= 1. && (4.1.4)
\end{aligned}$$

Moreover, (4.1.2) is tight if and only if $E_\lambda \mathbf{x}$ *and* $E_\lambda \mathbf{y}$ *are linearly dependent for each* $\lambda \in \Phi_{\mathbf{x}}$ *(equivalently,* $E_\lambda \mathbf{x}$ *and* $E_\lambda \mathbf{y}$ *are parallel vectors for each* $\lambda \in \Phi_{\mathbf{x}}$*), while (4.1.3) tight if and only if* $\|E_\lambda \mathbf{x}\| = \|E_\lambda \mathbf{y}\|$ *for each* $\lambda \in \Phi_{\mathbf{x}}$.

Proof. Let $M = \sum_{\lambda \in \mathrm{spec}(M)} \lambda E_\lambda$ be the spectral decomposition of M. Using the fact that $\mathbf{y}^* E_\lambda \mathbf{x} = (E_\lambda \mathbf{y})^*(E_\lambda \mathbf{x})$, we may write

$$\frac{1}{\|\mathbf{x}\|^2}|\mathbf{y}^* U(t)\mathbf{x}| = \frac{1}{\|\mathbf{x}\|^2}\left|\sum_{\lambda \in \Phi_{\mathbf{x}}} e^{\mathrm{i}t\lambda} \mathbf{y}^* E_\lambda \mathbf{x}\right| = \frac{1}{\|\mathbf{x}\|^2}\left|\sum_{\lambda \in \Phi_{\mathbf{x}}} e^{\mathrm{i}t\lambda} (E_\lambda \mathbf{y})^*(E_\lambda \mathbf{x})\right|. \qquad (4.1.5)$$

Applying the triangle inequality yields (4.1.1). Next, we invoke the Cauchy-Schwarz inequality to obtain (4.1.2) and (4.1.3) from (4.1.1) and (4.1.2), respectively. Finally, using the fact that $\|E_\lambda \mathbf{y}\|^2 = (E_\lambda \mathbf{y})^*(E_\lambda \mathbf{y}) = \mathbf{y}^* E_\lambda \mathbf{y}$ and $\sum_{\lambda \in \Phi_{\mathbf{x}}} E_\lambda \mathbf{y} = \mathbf{y}$ gives us

$$\sum_{\lambda \in \Phi_{\mathbf{x}}} \|E_\lambda \mathbf{y}\|^2 = \sum_{\lambda \in \Phi_{\mathbf{x}}} \mathbf{y}^* E_\lambda \mathbf{y} = \mathbf{y}^* \sum_{\lambda \in \Phi_{\mathbf{x}}} E_\lambda \mathbf{y} = \mathbf{y}^* \mathbf{y} = \|\mathbf{y}\|^2 = \|\mathbf{x}\|^2.$$

So (4.1.4) follows from (4.1.3). The rest is due to the Cauchy-Schwarz inequality. □

Lemma 4.1.2 yields the following characterisation of PST.

Theorem 4.1.3. *Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ *and phase factor* γ *if and only if both conditions below hold.*

1. $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral, that is, for each* $\lambda \in \Phi_{\mathbf{x}}$, *we have* $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ *for some unit complex number* ζ_λ.
2. $\gamma = e^{\mathrm{i}\tau\lambda}\zeta_\lambda = e^{\mathrm{i}\tau\theta}\zeta_\theta$ *for any* $\lambda, \theta \in \Phi_{\mathbf{x}}$.

Proof. Suppose perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ. By Lemma 4.1.1, this is the same as saying that $\frac{1}{\|\mathbf{x}\|^2}|\mathbf{y}^* U(\tau)\mathbf{x}| = 1$. Equivalently, every inequality in

Lemma 4.1.2 is an equality at time τ. Note that (4.1.2) and (4.1.3) are simultaneously tight if and only if $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ for each $\lambda \in \Phi_{\mathbf{x}}$, where ζ_λ is a unit complex number. That is, $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral. This proves 1. Using the strong cospectrality property, we may write (4.1.5) as

$$\frac{1}{\|\mathbf{x}\|^2}|\mathbf{y}^* U(t)\mathbf{x}| = \frac{1}{\|\mathbf{x}\|^2}\left|\sum_{\lambda\in\Phi_{\mathbf{x}}} e^{it\lambda}\zeta_\lambda (E_\lambda \mathbf{y})^*(E_\lambda \mathbf{y})\right|.$$

Therefore, (4.1.1) is tight if and only if 2 holds. The converse is straightforward. □

Corollary 4.1.4. *If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *with* $E_\lambda \mathbf{x} = e^{\mathrm{i}\mu_\lambda} E_\lambda \mathbf{y}$ *for each* $\lambda \in \Phi_{\mathbf{x}}$*, then*

$$\frac{\lambda-\theta}{\alpha-\beta} = \frac{\mu_\theta - \mu_\lambda + 2\ell_{\lambda,\theta}\pi}{\mu_\beta - \mu_\alpha + 2\ell_{\alpha,\beta}\pi} \tag{4.1.6}$$

for any $\lambda, \theta, \alpha, \beta \in \Phi_{\mathbf{x}}$ *with* $\alpha \neq \beta$ *and for some integers* $\ell_{\lambda,\theta}, \ell_{\alpha,\beta}$*.*

Proof. From Theorem 4.1.3(2), we have $e^{\mathrm{i}\tau\lambda}e^{\mathrm{i}\mu_\lambda} = e^{\mathrm{i}\tau\theta}e^{\mathrm{i}\mu_\theta}$ for any $\lambda, \theta \in \Phi_{\mathbf{x}}$. That is, $e^{\mathrm{i}\tau(\lambda-\theta)} = e^{\mathrm{i}(\mu_\theta-\mu_\lambda)}$. Equivalently, $\tau = \frac{\mu_\theta-\mu_\lambda+2\ell_{\lambda,\theta}\pi}{\lambda-\theta}$ for some integer $2\ell_{\lambda,\theta}$. Similarly, if $\alpha, \beta \in \Phi_{\mathbf{x}}$, then $\tau = \frac{\mu_\beta-\mu_\alpha+2\ell_{\alpha,\beta}\pi}{\alpha-\beta}$ for some integer $2\ell_{\alpha,\beta}$. Thus,

$$\frac{\mu_\theta - \mu_\lambda + 2\ell_{\lambda,\theta}\pi}{\lambda-\theta} = \frac{\mu_\beta - \mu_\alpha + 2\ell_{\alpha,\beta}\pi}{\alpha-\beta}$$

from which our result follows. □

Remark 4.1.5. The right-hand side of (4.1.6) need not be rational for any $\lambda, \theta, \alpha, \beta \in \Phi_{\mathbf{x}}$ with $\alpha \neq \beta$. Equivalently, $\Phi_{\mathbf{x}} = \Phi_{\mathbf{y}}$ need not satisfy the ratio condition, and so $\mathbf{x}, \mathbf{y}$ need not be periodic by Theorem 3.7.3. Consequently, PST involving pure states need not imply periodicity. Indeed, if we take $\mathbf{x} \in \mathbb{C}^n$ that is not a fixed state such that $\Phi_{\mathbf{x}}$ does not satisfy the ratio condition, then PST occurs from $\mathbf{x}$ and $U(t)\mathbf{x}$ for any time t, but $\mathbf{x}$ is not periodic in this case.

We now provide a necessary condition such that PST implies periodicity.

Theorem 4.1.6. *Suppose perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$*. If* $E_\lambda \mathbf{x} = e^{\mathrm{i}\mu_\lambda} E_\lambda \mathbf{y}$ *for each* $\lambda \in \Phi_{\mathbf{x}}$ *and each* μ_λ *is a rational multiple of* π*, then* $\Phi_{\mathbf{x}} = \Phi_{\mathbf{y}}$ *satisfies the ratio condition. Equivalently,* $\mathbf{x}$ *and* $\mathbf{y}$ *are periodic pure states.*

Proof. Our assumption implies that the right-hand side of (4.1.6) is rational for any $\lambda, \theta, \alpha, \beta \in \Phi_{\mathbf{x}}$ with $\alpha \neq \beta$. Equivalently, $\Phi_{\mathbf{x}} = \Phi_{\mathbf{y}}$ satisfies the ratio condition. □

Remark 4.1.7. By Theorem 3.7.3, we may restate Theorem 4.1.6 as: if PST occurs from $\mathbf{x}$ to $\mathbf{y}$, and $\mathbf{x}, \mathbf{y}$ are m-strongly cospectral, then $\mathbf{x}, \mathbf{y}$ are periodic.

From Remark 4.1.5, we know that PST in general need not imply periodicity. Nonetheless, for m-strongly cospectral pure states, PST implies periodicity by Remark 4.1.7. This property makes the class of m-strongly cospectral pure states special. It also generalises the fact that the existence of PST from a real pure state to another implies periodicity of the real pure states involved (such pure states are 2-strongly cospectral by Remark 3.5.4).

4.2 Minimum PST time

We now establish some fundamental results about the minimum PST time.

Theorem 4.2.1. *If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$*, then the minimum PST time always exists.*

Proof. By way of contradiction, suppose PST occurs from $\mathbf{x}$ to $\mathbf{y}$ and no minimum PST time exists. If $\tau_1 > 0$ is a PST time, then we can find another PST time τ_2 with $0 < \tau_2 < \tau_1$. Arguing inductively, we build a sequence $\{\tau_k\}$ of positive PST times such that $\lim_{k\to\infty} \tau_k = \tau$ for some $\tau \in \mathbb{R}$. Consider the function $f : \mathbb{R} \to \mathbb{R}$ given by $f(t) = \frac{1}{\|\mathbf{y}\|^2}|\mathbf{y}^* U(t)\mathbf{x}|$, which is continuous. Because PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at each time τ_k, Lemma 4.1.1 gives us

$$f(\tau_k) = \frac{1}{\|\mathbf{y}\|^2}|\mathbf{y}^* U(\tau_k)\mathbf{x}| = 1.$$

Since f is continuous, we obtain

$$\frac{1}{\|\mathbf{y}\|^2}|\mathbf{y}^* U(\tau)\mathbf{x}| = f(\tau) = f(\lim_{k\to\infty} \tau_k) = \lim_{k\to\infty} f(\tau_k) = 1.$$

Equivalently, PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ by Lemma 4.1.1. Since $\tau < \tau_k$ for all k, it follows that τ is a minimum PST time, a contradiction. □

The same argument above can be used to show that the minimum period of a periodic pure state always exists.

Theorem 4.2.2. *Let* $\mathbf{x}$ *be periodic with minimum period* ρ*. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *with minimum PST time* τ*, then* $\mathbf{y}$ *is also periodic and perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* $\tau + q\rho$ *for all integers* q*.*

Proof. The assumption implies that $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral, and hence they have the same eigenvalue supports. Also, $\mathbf{y}$ is periodic. Now, if γ and ζ are the phase factors for periodicity and PST at times ρ and τ, then

$$U(\tau+q\rho)\mathbf{x} = U(\tau)U(\rho)^q\mathbf{x} = \gamma^q U(\tau)\mathbf{x} = \gamma^q\zeta\mathbf{y}.$$

Thus, PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time $\tau+q\rho$ for all integers q. $\square$

The following result complements Remark 4.1.7.

Theorem 4.2.3. *Let* $\mathbf{x},\mathbf{y}\in\mathbb{C}^n$ *be* m*-strongly cospectral. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ*, then* $\mathbf{x}$ *and* $\mathbf{y}$ *are periodic at time* $m\tau$*.*

Proof. If PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ, then $e^{\mathrm{i}\tau\lambda}e^{\mathrm{i}2\pi\ell_\lambda/m} = e^{\mathrm{i}\tau\theta}e^{\mathrm{i}2\pi\ell_\theta/m}$ by Theorem 4.1.3(2). That is,

$$e^{\mathrm{i}m\tau\lambda} = (e^{\mathrm{i}\tau\lambda}e^{\mathrm{i}2\pi\ell_\lambda/m})^m = (e^{\mathrm{i}\tau\theta}e^{\mathrm{i}2\pi\ell_\theta/m})^m = e^{\mathrm{i}m\tau\theta}, \tag{4.2.1}$$

and so for all $\lambda,\theta\in\Phi_{\mathbf{x}}$, we have $m\tau(\lambda-\theta)\equiv 0 \pmod{2\pi}$. Equivalently, $\Phi_{\mathbf{x}}=\Phi_{\mathbf{y}}$ satisfies the ratio condition, and so Theorem 3.7.3 implies that $\mathbf{x},\mathbf{y}$ are periodic. $\square$

Corollary 4.2.4. *Let* $\mathbf{x},\mathbf{y}\in\mathbb{C}^n$ *be* m*-strongly cospectral. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *with minimum PST time* τ*, then* $\mathbf{x}$ *and* $\mathbf{y}$ *are both periodic at time* $k\tau$ *for any integer* $k\equiv 0 \pmod{m}$*, and perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* $\ell\tau$ *for any integer* $\ell\equiv 1 \pmod{m}$*.*

Proof. If PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ, say with phase factor γ, then Theorem 4.2.3 implies that $\mathbf{x},\mathbf{y}$ are periodic at time $m\tau$, say with phase factor ζ. By Remark 3.7.6, $\mathbf{x},\mathbf{y}$ are periodic at time $qm\tau$ with phase factor ζ^q for each integer $q>0$. Taking $k=qm$ yields the first statement in the conclusion. For the second statement, let $\ell=qm+1$. Then $\ell\equiv 1 \pmod{m}$ and

$$U(\ell\tau)\mathbf{x} = U(\tau)U(m\tau)^q\mathbf{x} = \zeta^q U(\tau)\mathbf{x} = (\zeta^q\gamma)\mathbf{y}.$$

Equivalently, there is PST from $\mathbf{x}$ to $\mathbf{y}$ at time $\ell\tau$ with phase factor $\zeta^q\gamma$. $\square$

Remark 4.2.5. From Corollary 4.2.4, it is immediate that if PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ, where τ is not necessarily the minimum PST time, then perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ at time $\ell\tau$ for any integer $\ell\equiv 1 \pmod{m}$.

4.3 Symmetry

For real pure states, it was observed that PST is a *symmetric* relation. That is, if PST occurs from $\mathbf{x}$ to $\mathbf{y}$, then PST also occurs from $\mathbf{y}$ to $\mathbf{x}$ at the same time with the same phase factor. The following result states that for pure states in general, this symmetry property only happens to pure states that are 2-strongly cospectral.

Theorem 4.3.1. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$*. Perfect state transfer from* $\mathbf{x}$ *to* $\mathbf{y}$ *is symmetric if and only if* $\mathbf{x}$ *and* $\mathbf{y}$ *are* 2*-strongly cospectral.*

Proof. Suppose perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$, and from $\mathbf{y}$ to $\mathbf{x}$ at the same time τ with the same phase factor γ. Then by Theorem 4.1.3(2), we have

$$\gamma = e^{\mathrm{i}\tau\lambda}\zeta_\lambda = e^{\mathrm{i}\tau\theta}\zeta_\theta \quad \text{and} \quad \gamma = e^{\mathrm{i}\tau\lambda}\overline{\zeta_\lambda} = e^{\mathrm{i}\tau\theta}\overline{\zeta_\theta}$$

for any $\lambda, \theta \in \Phi_{\mathbf{x}}$. Thus, $\zeta_\lambda = \overline{\zeta_\lambda}$ for any $\lambda \in \Phi_{\mathbf{x}}$, and so $\zeta_\lambda = \pm 1$. Conversely, if $\mathbf{x}$ and $\mathbf{y}$ are 2-strongly cospectral, then $E_\lambda \mathbf{x} = \zeta_\lambda E_\lambda \mathbf{y}$ for each $\lambda \in \Phi_{\mathbf{x}}$ where $\zeta_\lambda = \pm 1$. Equivalently, $E_\lambda \mathbf{y} = \zeta_\lambda E_\lambda \mathbf{x}$. Now, if perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ phase factor γ, then by Theorem 4.1.3(2), we have $\gamma = e^{\mathrm{i}\tau\lambda}\zeta_\lambda = e^{\mathrm{i}\tau\theta}\zeta_\theta$ for any $\lambda, \theta \in \Phi_{\mathbf{x}}$, which is the condition needed for PST to occur from $\mathbf{y}$ to $\mathbf{x}$. □

We show that a weaker version of the symmetry property holds for all pure states.

Lemma 4.3.2. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$*. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ *and phase factor* γ*, then it also occurs from* $\mathbf{y}$ *to* $\mathbf{x}$ *at time* $-\tau$ *and phase factor* $\overline{\gamma}$*.*

Proof. Multiplying both sides of $U(t)\mathbf{x} = \gamma\mathbf{y}$ by $\overline{\gamma}U(-t)$ yields $U(-t)\mathbf{y} = \overline{\gamma}\mathbf{x}$. □

If $\tau > 0$, then the PST from $\mathbf{y}$ to $\mathbf{x}$ in the conclusion of Lemma 4.3.2 occurs at a negative time, since $-\tau < 0$. Nonetheless, Theorem 4.2.1 guarantees that there is a minimum PST time from $\mathbf{y}$ to $\mathbf{x}$ that is positive. For m-strongly cospectral pure states, one can derive the minimum PST time from $\mathbf{y}$ to $\mathbf{x}$ from the minimum PST time from $\mathbf{x}$ to $\mathbf{y}$.

Theorem 4.3.3. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ *be* m*-strongly cospectral. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ *and phase factor* γ*, then perfect state transfer occurs from* $\mathbf{y}$ *to* $\mathbf{x}$ *at time* $(m-1)\tau$ *and phase factor* $\gamma^{-1}\zeta$*, where* ζ *is the phase factor at the period* $m\tau$ *of* $\mathbf{x}$*.*

Proof. Since $\mathbf{x}, \mathbf{y}$ are m-strongly cospectral, Theorem 4.2.3 implies that $\mathbf{x}, \mathbf{y}$ are periodic at time $m\tau$ with phase factor, say ζ. By Lemma 4.3.2, there is PST from $\mathbf{y}$ to $\mathbf{x}$ at time $-\tau$ and phase factor $\overline{\gamma}$. Invoking Remark 4.2.5, there is also PST from $\mathbf{y}$ to $\mathbf{x}$ at time $-\ell\tau$ for any integer $k \equiv 1 \pmod{m}$. In this case, $-\ell \equiv m - 1 \pmod{m}$. Thus, there is PST from $\mathbf{y}$ to $\mathbf{x}$ at time $(m-1)\tau > 0$ with phase factor $\gamma^{-1}\zeta$ because $U((m-1)\tau)\mathbf{x} = U(m\tau)U(-\tau)\mathbf{x} = \gamma^{-1}U(m\tau)\mathbf{y} = \gamma^{-1}U(\rho)\mathbf{y} = \gamma^{-1}\zeta\mathbf{y}$. □

We end this section with the following important remark.

Remark 4.3.4. By virtue of Lemma 4.3.2, PST from $\mathbf{x}$ to $\mathbf{y}$ implies PST from $\mathbf{y}$ to $\mathbf{x}$, and the minimum PST times for both need not be equal. From this fact, if we want to specify the minimum PST time in a given statement, then we say 'PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ', but if the PST time is not important, then we simply say PST from $\mathbf{x}$ to $\mathbf{y}$. Moreover, if $\mathbf{x}$ and $\mathbf{y}$ are 2-strongly cospectral, then Theorem 4.3.1 allows us to say 'PST occurs between $\mathbf{x}$ and $\mathbf{y}$ at time τ' in lieu of 'PST occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ'.

4.4 Monogamy

For real pure states, PST is known to be a *monogamous* relation. That is, if there is PST from $\mathbf{x}$ to $\mathbf{y}$, and there is also PST from $\mathbf{x}$ to $\mathbf{z}$, then $\mathbf{y} = \pm\mathbf{z}$ (equivalently, $\mathbf{y} \in \operatorname{span}\{\mathbf{z}\}$). However, PST on complex pure states need not obey monogamy. Indeed, if $\mathbf{x}$ is not a fixed state, then there is PST from $\mathbf{x}$ to $U(t)\mathbf{x}$ for all $t > 0$. In this case, there exist at least two times $t_1, t_2 \in \mathbb{R}$ with $t_1 \neq t_2$ such that $U(t_1)\mathbf{x}$ and $U(t_2)\mathbf{x}$ are linearly independent. Otherwise, $U(t)\mathbf{x} \in \operatorname{span}\{\mathbf{z}\}$ for all $t \in \mathbb{R}$, and so Proposition 3.3.3(3) implies that $\mathbf{x}$ is a fixed state, a contradiction.

In this subsection, our goal is to show that PST on m-strongly cospectral pure states is monogamous if and only if $m = 2$. To do this, we need the following result.

Proposition 4.4.1. *Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. If perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$, and from $\mathbf{x}$ to $\mathbf{z}$ at the same time, then $\mathbf{y} = \eta\mathbf{z}$ for some unit complex number η.*

Proof. By assumption, we have $U(\tau)\mathbf{x} = \gamma\mathbf{y}$ and $U(\tau)\mathbf{x} = \zeta\mathbf{z}$ for some unit complex numbers γ, ζ. Thus, $\gamma\mathbf{y} = \zeta\mathbf{z}$, and so the conclusion is immediate. ☐

Theorem 4.4.2. *Let $m \geq 2$ and $\mathbf{x} \in \mathbb{C}^n$. Fix an $|\Phi_{\mathbf{x}}|$-tuple $(\ell_\lambda)_{\lambda\in\Phi_{\mathbf{x}}}$ of integers from $\mathbb{Z}_m$ such that (ℓ_λ) has at least two distinct entries and $\gcd(\ell_\lambda, m) = 1$ for at least one λ. For each $k \in \mathbb{Z}_m$, let*

$$\mathbf{y}_k = \sum_{\lambda\in\Phi_{\mathbf{x}}} e^{-\mathrm{i}2\pi(k\ell_\lambda)/m}\mathbf{u}_\lambda$$

where each $\mathbf{u}_\lambda$ is an eigenvector of λ and $\mathbf{x} = \mathbf{y}_0$. The following are equivalent.

1. *For some $k \in \mathbb{Z}_m$, perfect state transfer occurs from $\mathbf{y}_k$ to $\mathbf{y}_{k+1}$ with minimum PST time τ.*

2. *For all $k \in \mathbb{Z}_m$, perfect state transfer occurs from $\mathbf{y}_k$ to $\mathbf{y}_{k+1}$ at the same minimum time τ and phase factor γ.*

3. *For some* $k, s \in \mathbb{Z}_m$ *with* $s \neq k$*, perfect state transfer occurs from* $\mathbf{y}_k$ *to* $\mathbf{y}_s$ *with minimum PST time* $(s-k)\tau$ *and phase factor* γ^{s-k} *whenever* $s > k$ *and* $(m-(s-k))\tau$ *and* $\gamma^{m-(s-k)}$ *otherwise.*

4. *For all* $k, s \in \mathbb{Z}_m$ *with* $s \neq k$*, perfect state transfer occurs from* $\mathbf{y}_k$ *to* $\mathbf{y}_s$ *with minimum PST time* $(s-k)\tau$ *and phase factor* γ^{s-k} *whenever* $s > k$ *and* $(m-(s-k))\tau$ *and* $\gamma^{m-(s-k)}$ *otherwise.*

Moreover, if one of the above statements hold, then each $\mathbf{y}_k$ *is periodic with* $\rho = m\tau$*.*

Proof. We first show that $\mathbf{y}_k$ and $\mathbf{y}_s$ are linearly independent for $k \neq s$. Let $\alpha, \beta \in \mathbb{C}$ such that $\alpha\mathbf{y}_k + \beta\mathbf{y}_s = \mathbf{0}$. Then $\sum_{\lambda\in\Phi_{\mathbf{x}}} \left(\alpha + \beta e^{-\mathrm{i}2\pi((s-k)\ell_\lambda)/m}\right)\mathbf{u}_\lambda = \mathbf{0}$. Since the $\mathbf{u}_\lambda$'s are linearly independent, $\alpha = -\beta e^{-\mathrm{i}2\pi((s-k)\ell_\lambda)/m}$ for all $\lambda \in \Phi_{\mathbf{x}}$. Since $\mathbf{x}$ is not fixed, we have $|\Phi_{\mathbf{x}}| \geq 2$. Since (ℓ_λ) has at least two distinct entries, the preceding equation only holds if and only if $\alpha = \beta = 0$. Thus, $\mathbf{y}_k$ and $\mathbf{y}_s$ are linearly independent.

To prove the equivalence of 1 and 2, it suffices to show 1 ⇒ 2. For each $k \in \mathbb{Z}_m$, $\mathbf{y}_k$ and $\mathbf{y}_{k+1}$ are strong cospectral by Theorem 3.5.12 with $E_\lambda\mathbf{y}_k = e^{\mathrm{i}2\pi\ell_\lambda/m}E_\lambda\mathbf{y}_{k+1}$. So, Theorem 4.1.3(1) holds for the pair $\{\mathbf{y}_k, \mathbf{y}_{k+1}\}$ for each $k \in \mathbb{Z}_m$. Since there is PST from $\mathbf{y}_j$ to $\mathbf{y}_{j+1}$ for some j, Theorem 4.1.3(2) yields $e^{\mathrm{i}\tau\lambda}e^{\mathrm{i}2\pi\ell_\lambda/m} = e^{\mathrm{i}\tau\theta}e^{\mathrm{i}2\pi\ell_\theta/m}$ for all $\lambda, \theta \in \Phi_{\mathbf{x}}$. But since this equation applies to each pair $\{\mathbf{y}_k, \mathbf{y}_{k+1}\}$, it follows that Theorem 4.1.3(2) also holds for the pair $\{\mathbf{y}_k, \mathbf{y}_{k+1}\}$ for each $k \in \mathbb{Z}_m$. Hence, we get PST from $\mathbf{y}_k$ to $\mathbf{y}_{k+1}$ for each k, and the PST times and phase factors are the same for all $k \in \mathbb{Z}_m$.

To prove the equivalence of 2 and 4, it suffices to show 2 ⇒ 4. By assumption, we may let $U(\tau)\mathbf{y}_k = \gamma\mathbf{y}_{k+1}$ for each $k \in \mathbb{Z}_m$. If $s > k$, then

$$U((s-k)\tau)\mathbf{y}_k = U(\tau)^{s-k}\mathbf{y}_k = \gamma^{s-k}\mathbf{y}_{k+(s-k)} = \gamma^{s-k}\mathbf{y}_s.$$

The case $s < k$ follows similarly. From this, we get PST from $\mathbf{x}$ to $\mathbf{y}_k$ at time $k\tau$ for all $k \in \mathbb{Z}_m\backslash\{0\}$. Now, suppose there is some $0 < \tau' < (s-k)\tau$ such that PST occurs from $\mathbf{y}_k$ to $\mathbf{y}_s$ at time τ'. Using the same argument as above, we get that $\mathbf{y}_k$ is periodic at $m\tau'$. By Theorem 3.7.8, $m\tau'$ is an integer multiple of $\rho = m\tau$, and so τ' is an integer multiple of τ. Therefore, $\tau' = j\tau$ for some $j \in \{1, \ldots, s-k-1\}$, in which case PST occurs from $\mathbf{y}_k$ to $\mathbf{y}_{k+j}$ at time τ', where $\mathbf{y}_{k+j} \neq \mathbf{y}_s$ and $\mathbf{y}_{k+j}$ and $\mathbf{y}_s$ are linearly independent. Since PST also occurs $\mathbf{y}_k$ to $\mathbf{y}_s$ at time τ', Proposition 4.4.1 implies that $\mathbf{y}_{k+j}$ and $\mathbf{y}_s$ are linearly dependent, a contradiction. This shows that $(s-k)\tau$ is the minimum PST time from $\mathbf{y}_k$ to $\mathbf{y}_s$. Similarly, for the case $s < k$.

The proof of 3 ⇒ 4 is similar to that of 1 ⇒ 2, while 4 ⇒ 3 is straightforward. Thus, 3 and 4 are equivalent.

Finally, to establish $\rho = m\tau$, suppose the minimum PST time from $\mathbf{y}_k$ to $\mathbf{y}_{k+1}$ is τ. If one of 1-4 holds, then the above equivalence yields 2, in which case Theorem 4.2.3 implies that $\mathbf{y}_k$ is periodic at time $m\tau$. Here, we prove that $\rho = m\tau$. From (4.2.1), we obtain

$$m\tau(\lambda - \theta) \equiv 0 \pmod{2\pi}$$

for all $\lambda, \theta \in \Phi_{\mathbf{x}}$ Invoking (3.7.8), the minimum period of $\mathbf{y}_k$ is $\rho = \frac{2\pi q}{|\lambda_1 - \lambda_2|}$, for some fixed $\lambda_1, \lambda_2 \in \Phi_{\mathbf{x}}$ with $\lambda_1 \neq \lambda_2$. By Remark 3.7.9, the least $\tau > 0$ such that $m\tau(\lambda - \theta)$ is an integer multiple of 2π for any $\lambda, \theta \in \Phi_{\mathbf{x}}$ is $\tau = \frac{2\pi q}{m|\lambda_1 - \lambda_2|}$. Therefore, $\rho = m\tau$. $\square$

The following is immediate from Theorem 4.4.2(3,4) and the fact that $\mathbf{x} = \mathbf{y}_0$.

Corollary 4.4.3. *Perfect state transfer from* $\mathbf{x}$ *to* $\mathbf{y}_k$ *at time* $k\tau$ *and phase factor* γ^k *for some* $k \in \mathbb{Z}_m \backslash \{0\}$ *if and only if it holds for all* $k \in \mathbb{Z}_m \backslash \{0\}$.

Corollary 4.4.4. *Suppose in addition that* $(l_\lambda)_{\lambda \in \Phi_{\mathbf{x}}}$ *is another* $|\Phi_{\mathbf{x}}|$*-tuple with the same property as* $(\ell)_\lambda$ *in Theorem 4.4.2. For each* $j \in \mathbb{Z}_m$, *let*

$$\mathbf{z}_j = \sum_{\lambda \in \Phi_{\mathbf{x}}} e^{-\mathrm{i}2\pi(jl_\lambda)/m} \mathbf{u}_\lambda.$$

If there is perfect state transfer from $\mathbf{x}$ *to* $\mathbf{y}_k$ *and from* $\mathbf{x}$ *to* $\mathbf{z}_j$ *for some* $j, k \in \mathbb{Z}_m \backslash \{0\}$, *then* $\{\mathbf{y}_j, \mathbf{z}_j\}$ *is a linearly dependent set for each* $j \in \mathbb{Z}_m$.

Proof. Suppose there is perfect state transfer from $\mathbf{x} = \mathbf{z}_0$ to $\mathbf{z}_j$, and $\mathbf{x} = \mathbf{y}_0$ to $\mathbf{y}_k$ for some $j, k \in \mathbb{Z}_m \backslash \{0\}$. Then by Theorem 4.4.2(4), there is PST from $\mathbf{x}$ to $\mathbf{z}_j$, and from $\mathbf{x}$ to $\mathbf{y}_j$ with minimum PST time $j\tau$ and phase factor γ^j for all $j \in \mathbb{Z}_m \backslash \{0\}$. By Proposition 4.4.1, $\mathbf{y}_j$ and $\mathbf{z}_j$ are linearly dependent for all $j \in \mathbb{Z}_m$. $\square$

Corollary 4.4.5. *Perfect state transfer occurs on* m*-strongly cospectral pure states is monogamous if and only if* $m = 2$.

Proof. If $m \geq 3$, then PST on m-strongly cospectral pure states is non-monogamous by Corollary 4.4.3. Now, let $\mathbf{x}$ be 2-strongly cospectral with $\mathbf{y}$ and $\mathbf{z}$. If we have PST from $\mathbf{x}$ to $\mathbf{y}$ and from $\mathbf{x}$ to $\mathbf{y}_z$, then Theorem 4.4.2(2) and Corollary 4.4.4 implies that $\mathbf{y}_1$ and $\mathbf{y}_2$ are linearly dependent. In this case, PST is monogamous. $\square$

Theorem 4.4.2 also reveals a cyclic behaviour of PST on $\mathcal{B} = (\mathbf{x} = \mathbf{y}_0, \mathbf{y}_1, \ldots, \mathbf{y}_{m-1})$, which we call a *PST block* relative to the $|\Phi_{\mathbf{x}}|$-tuple (ℓ_λ). Note that a PST block for m-strongly cospectral pure states always has size m. If $\mathcal{B}' = (\mathbf{x} = \mathbf{z}_0, \mathbf{z}_1, \ldots, \mathbf{z}_{m-1})$ is another PST block that involves $\mathbf{x}$ relative to another $|\Phi_{\mathbf{x}}|$-tuple (l_λ), then Corollary 4.4.4 implies that the vectors in each coordinate of $\mathcal{B}$ and $\mathcal{B}'$, which are $\mathbf{y}_j$ and

$\mathbf{z}_j$, are linearly dependent for each $j \in \mathbb{Z}_m$. This shows that a pure state involved in m-strong cospectrality belongs to at most one PST block (up to 'coordinate-wise' linear independence of blocks). This in turn implies that the assignment of a pure state involved in m-strong cospectrality to a PST block is monogamous. Moreover, this important observation allows us to view PST on m-strongly cospectral pure states as an equivalence relation with the PST blocks as equivalence classes.

4.5 PST when $|\Phi_{\mathbf{x}}| = 2$

It is known that if $n \geq 3$, then vertex states that admit PST have eigenvalue supports of size at least three [74, Theorem 3.4]. This follows from the fact that PST between vertex states $\mathbf{e}_u$ and $\mathbf{e}_v$ implies that $|\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}| \geq 2$ and $|\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}| \geq 1$. For pure states in general, this need not be the case. In this section, we examine the properties of pure states admitting PST with eigenvalue supports of size two.

Corollary 4.5.1. *Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ with $\Phi_{\mathbf{x}} = \{\lambda_1, \lambda_2\}$.Perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ if and only if they are strongly cospectral. In particular, if $E_j\mathbf{x} = e^{\mathrm{i}\mu_j} E_j\mathbf{y}$ for some $\mu_j \in [0, 2\pi)$, then the minimum PST time is $\tau = \frac{\mu_2-\mu_1+2k_0\pi}{|\lambda_1-\lambda_2|}$, where $k_0 = 1$ if $\mu_2 - \mu_1$ and $\lambda_1 - \lambda_2$ have opposite signs and $k_0 = 0$ otherwise.*

Proof. Since $\Phi_{\mathbf{x}} = \{\lambda_1, \lambda_2\}$, Proposition 3.3.2 allows us to write $\mathbf{x} = \mathbf{u}_1 + \mathbf{u}_2$, where each $\mathbf{u}_j$ is an eigenvector associated with an eigenvalue $\lambda_j \in \Phi_{\mathbf{x}}$. By Theorem 3.5.12, $\mathbf{x}, \mathbf{y}$ are strongly cospectral if and only if $\mathbf{y} = \overline{\zeta_1}\mathbf{u}_1 + \overline{\zeta_2}\mathbf{u}_2$, in which case $E_j\mathbf{x} = \zeta_j E_j\mathbf{y}$ for each j. If we write $\zeta_j = e^{\mathrm{i}\mu_j}$ for some $\mu_j \in [0, 2\pi)$, then $\mu_1 \neq \mu_2$ by Remark 3.5.2. In this case, $e^{\mathrm{i}\tau\lambda_1}\zeta_1 = e^{\mathrm{i}\tau\lambda_2}\zeta_2$ holds at time $\tau = \frac{\mu_2-\mu_1+2k\pi}{\lambda_1-\lambda_2}$ for all integers k. Thus, the above corollary holds by Theorem 4.1.3. □

Remark 4.5.2. In the proof of Corollary 4.5.1, if each $\mathbf{u}_j$ is a real eigenvector for λ_j, and $\zeta_1 = -\zeta_2 = 1$, then we obtain real pure states $\mathbf{x}, \mathbf{y}$.

Remark 4.5.3. If $\mathbf{x} = \mathbf{e}_u$ and $\mathbf{y} = \mathbf{e}_v$ are strongly cospectral, then $|\Phi_{\mathbf{x}}| \geq 3$ by [74, Theorem 3.4] and so Corollary 4.5.1 does not apply to vertex states whenever $n \geq 3$.

Corollary 4.5.4. *If M has at least two distinct eigenvalues, then perfect state transfer occurs in a quantum walk relative to M.*

As M is an irreducible real symmetric matrix, it has at least two distinct eigenvalues. Thus, the following is immediate from Corollary 4.5.4 and Remark 4.5.2.

Corollary 4.5.5. *A quantum walk on an irreducible real symmetric matrix admits perfect state transfer between pure states. These pure states may be taken to be real.*

Since the Hamiltonian M respects the adjacencies in X, M is irreducible if and only if X is connected. Thus, the following is immediate from Corollary 4.5.5.

Corollary 4.5.6. *All connected graphs on $n \geq 2$ vertices admit perfect state transfer between pure states. These pure states may be taken to be real.*

Remark 4.5.7. Corollary 4.5.6 applies to any graph G that is not empty (that is, G has at least one edge) since such graph will have at least one connected component.

4.6 Prescribed PST

We now show that any periodic pure state admits PST.

Theorem 4.6.1. *Let $\mathbf{x} \in \mathbb{C}^n$ be periodic with minimum period ρ. For any integer $m \geq 2$, there exists $\mathbf{y} \in \mathbb{C}^n$ that is m-strongly cospectral with $\mathbf{x}$ and perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ at $\frac{\rho}{m}$.*

Proof. Let $m \geq 2$ and $\Phi_{\mathbf{x}} = \{\lambda_1, \dots, \lambda_r\}$ with $r \geq 2$. By Proposition 3.3.2, we may write $\mathbf{x} = \sum_{j=1}^{r} \mathbf{u}_j$, where each $\mathbf{u}_j$ is an eigenvector associated with an eigenvalue λ_j. If ρ is a period of $\mathbf{x}$, then at time ρ, the phase factor is $\gamma = e^{\mathrm{i}\rho\lambda_j}$ for each j by (3.7.2). By De Moivre's Theorem,

$$\gamma^{1/m} = e^{\mathrm{i}\rho\lambda_j/m} e^{\mathrm{i}2\pi\rho\ell_j/m} \quad \text{for any } \ell_j \in \mathbb{Z}_m. \tag{4.6.1}$$

For each j, choose an integer $\ell_j \in \mathbb{Z}_m$ such that $\gcd(\ell_j, m) = 1$ for at least one j and $\ell_j \neq \ell_k$ for at least two indices j, k. Let $\zeta_j := e^{\mathrm{i}2\pi\ell_j/m}$ and define $\mathbf{y} := \sum_{j=1}^{r} \overline{\zeta_j} \mathbf{u}_j$. By Theorem 3.5.12, $\mathbf{x}, \mathbf{y}$ are m-strongly cospectral. Combining this with (4.6.1) yields PST from $\mathbf{x}$ to $\mathbf{y}$ at $\frac{\rho}{m}$ by Theorem 4.1.3 with phase factor $\gamma^{1/m}$. □

Remark 4.6.2. In the proof of Theorem 4.6.1, if $\mathbf{x} \in \mathbb{R}^n$, we may take each $\mathbf{u}_j$ as a real eigenvector associated with λ_j, and $\zeta_j = \pm 1$, so that $\mathbf{y}$ is also real.

Theorem 4.6.1 implies that in a periodic graph, any pure state admits PST with another pure state to which it is m-strongly cospectral with.

Next, we establish that for any pure states $\mathbf{x}$ and $\mathbf{y}$, there is a Hermitian matrix H such that PST occurs from $\mathbf{x}$ to $\mathbf{y}$ relative to H. Recall that $A \circ B$ denotes the Schur product of matrices A and B.

Theorem 4.6.3. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$*. For all* $\tau > 0$*, for all unit complex number* γ *and for all integers* $2 \leq r \leq n$*, there exists a Hermitian matrix* M *such that* $|\Phi_{\mathbf{x}}| = r$ *and perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at time* τ *with phase factor* γ*.*

Proof. Let $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ and $\theta \in [0, 2\pi)$ be the angle such that $\mathbf{y}^*\mathbf{x} = e^{\mathrm{i}\theta}|\mathbf{y}^*\mathbf{x}|$. Fix a unit complex number $\gamma = e^{\mathrm{i}\mu}$ with $\mu \in [0, 2\pi)$, and an integer r such that $2 \leq r \leq n$. Choose real vectors $\mathbf{a} = [a_j], \mathbf{b} = [b_j], \mathbf{c} = [c_j], \mathbf{d} = [d_j] \in \mathbb{R}^r$ such that at least one of $\mathbf{a}, \mathbf{b}$ is nonzero, at least one of $\mathbf{c}, \mathbf{d}$ is nonzero, and

$$\mathbf{a} \circ \mathbf{c} + \mathbf{b} \circ \mathbf{d} = 0 \quad \text{and} \quad \mathbf{a}^T\mathbf{d} - \mathbf{b}^T\mathbf{c} = 0. \tag{4.6.2}$$

There are many such vectors. For example, one may take $\mathbf{a}, \mathbf{b}$ to be arbitrary vectors in $\mathbb{R}^r$ with $\mathbf{b}$ having all entries nonzero, and then choose $\mathbf{c}$ to be a real vector that is orthogonal to the vector $[\frac{a_1^2+b_1^2}{b_1}, \frac{a_2^2+b_2^2}{b_2}, \ldots, \frac{a_r^2+b_r^2}{b_r}]^T$, and $\mathbf{d}$ be a real vector such that $d_j = -\frac{a_j c_j}{b_j}$ for each j. Once the $\mathbf{a}, \mathbf{b}, \mathbf{c}, \mathbf{d}$ are chosen, define

$$\mathbf{z}_1 = \mathbf{a} + \mathbf{b}\mathrm{i} \quad \text{and} \quad \mathbf{z}_2 = \mathbf{c} + \mathbf{d}\mathrm{i} \tag{4.6.3}$$

which are nonzero complex vectors in $\mathbb{C}^r$. Since $\mathbf{a} \circ \mathbf{c} + \mathbf{b} \circ \mathbf{d} = 0$ by (4.6.2), it follows that $\mathbf{a}^T\mathbf{c} + \mathbf{b}^T\mathbf{d} = 0$. Combining this with $\mathbf{a}^T\mathbf{d} - \mathbf{b}^T\mathbf{c} = 0$ in (4.6.2), gives us

$$\mathbf{z}_1^*\mathbf{z}_2 = (\mathbf{a}^T - \mathbf{b}^T\mathrm{i})(\mathbf{c} + \mathbf{d}\mathrm{i}) = (\mathbf{a}^T\mathbf{c} + \mathbf{b}^T\mathbf{d}) + (\mathbf{a}^T\mathbf{d} - \mathbf{b}^T\mathbf{c})\mathrm{i} = 0.$$

Now, consider the complex vectors $\begin{bmatrix} \mathbf{z}_1 \\ \mathbf{0}_{n-r} \end{bmatrix}, \begin{bmatrix} \mathbf{z}_2 \\ \mathbf{0}_{n-r} \end{bmatrix} \in \mathbb{C}^n$, which are orthogonal because $\mathbf{z}_1^*\mathbf{z}_2 = 0$. Observe that

$$\{\mathbf{u}_1, \mathbf{u}_2\} := \left\{ \frac{1}{\|\mathbf{z}_1\|} \begin{bmatrix} \mathbf{z}_1 \\ \mathbf{0}_{n-r} \end{bmatrix}, \frac{1}{\|\mathbf{z}_2\|} \begin{bmatrix} \mathbf{z}_2 \\ \mathbf{0}_{n-r} \end{bmatrix} \right\} \tag{4.6.4}$$

and

$$\{\mathbf{v}_1, \mathbf{v}_2\} := \left\{ \frac{\mathbf{x} + e^{\mathrm{i}\theta}\mathbf{y}}{\|\mathbf{x} + e^{\mathrm{i}\theta}\mathbf{y}\|}, \frac{\mathbf{x} - e^{\mathrm{i}\theta}\mathbf{y}}{\|\mathbf{x} - e^{\mathrm{i}\theta}\mathbf{y}\|} \right\} \tag{4.6.5}$$

are orthonormal sets. So we may extend them to orthonormal bases $\mathcal{U} = \{\mathbf{u}_1, \ldots, \mathbf{u}_n\}$ and $\mathcal{V} = \{\mathbf{v}_1, \ldots, \mathbf{v}_n\}$ for $\mathbb{C}^n$, respectively. Then there exists a unitary matrix Q such that $Q\mathbf{u}_j = \mathbf{v}_j$ for each j. If we write $Q = [\mathbf{w}_1, \ldots, \mathbf{w}_n]$, where $\mathbf{w}_1, \ldots, \mathbf{w}_n$ are columns of Q, then the equations

$$Q\mathbf{u}_1 = \mathbf{v}_1 \quad \text{and} \quad Q\mathbf{u}_2 = \mathbf{v}_2$$

are equivalent to

$$\mathbf{x}+e^{\mathrm{i}\theta}\mathbf{y}=\gamma_1\sum_{j=1}^{r}\alpha_j\mathbf{w}_j \quad\text{and}\quad \mathbf{x}-e^{\mathrm{i}\theta}\mathbf{y}=\gamma_2\sum_{j=1}^{r}\beta_j\mathbf{w}_j,$$

where $\mathbf{z}_1=[\alpha_1,\ldots,\alpha_r,0,\ldots,0]^T$, $\mathbf{z}_1=[\beta_1,\ldots,\beta_r,0,\ldots,0]^T$, $\gamma_1=\frac{\|\mathbf{x}+e^{\mathrm{i}\theta}\mathbf{y}\|}{\|\mathbf{z}_1\|}$ and $\gamma_2=\frac{\|\mathbf{x}-e^{\mathrm{i}\theta}\mathbf{y}\|}{\|\mathbf{z}_2\|}$. Solving for $\mathbf{x}$ and $\mathbf{y}$ in the above equation gives us

$$\mathbf{x}=\frac{1}{2}\sum_{j=1}^{r}\left(\gamma_1\alpha_j+\gamma_2\beta_j\right)\mathbf{w}_j \tag{4.6.6}$$

and

$$\mathbf{y}=\frac{1}{2e^{\mathrm{i}\theta}}\sum_{j=1}^{r}\left(\gamma_1\alpha_j-\gamma_2\beta_j\right)\mathbf{w}_j. \tag{4.6.7}$$

Now, let

$$\overline{\zeta_j}:=\frac{\gamma_1\alpha_j-\gamma_2\beta_j}{e^{\mathrm{i}\theta}(\gamma_1\alpha_j+\gamma_2\beta_j)}.$$

Since $\mathbf{a}\circ\mathbf{c}+\mathbf{b}\circ\mathbf{d}=0$ from (4.6.2), we have $|\gamma_1\alpha_j+\gamma_2\beta_j|=|\gamma_1\alpha_j-\gamma_2\beta_j|$. Therefore, $|\zeta_j|=|\overline{\zeta_j}|=1$. Setting $\mathbf{u}_j:=\frac{1}{2}\left(\gamma_1\alpha_j+\gamma_2\beta_j\right)\mathbf{w}_j$, we obtain

$$\overline{\zeta_j}\mathbf{u}_j=\frac{1}{2e^{\mathrm{i}\theta}}\left(\gamma_1\alpha_j-\gamma_2\right)\mathbf{w}_j,$$

in which case, we may rewrite $\mathbf{x}$ and $\mathbf{y}$ in (4.6.6) and (4.6.7) as

$$\mathbf{x}=\sum_{j=1}^{r}\mathbf{u}_j \quad\text{and}\quad \mathbf{y}=\sum_{j=1}^{r}\overline{\zeta_j}\mathbf{u}_j. \tag{4.6.8}$$

Now, let $\{\lambda_1,\ldots,\lambda_n\}$ be a set of n distinct real numbers and consider the Hermitian matrix

$$M=\sum_{j=1}^{n}\lambda_j\mathbf{w}_j\mathbf{w}_j^*. \tag{4.6.9}$$

Since (4.6.8) holds, Theorem 3.5.12 implies that $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral relative to M with $E_j\mathbf{x}=\zeta_jE_j\mathbf{y}$ for each $j\in\{1,\ldots,r\}$ and $E_\ell\mathbf{x}=\mathbf{0}$ for $\ell\notin\{1,\ldots,r\}$. Therefore, $|\Phi_{\mathbf{x}}|=r$. Finally, if we let $\zeta_j=e^{\mathrm{i}\theta_j}$ where $\theta_j\in[0,2\pi)$, then we may each choose λ_j such that $\lambda_j\tau\equiv\mu-\theta_j \pmod{2\pi}$. In this case, we get

$$\gamma=e^{\mathrm{i}\mu}=e^{\mathrm{i}(t\lambda_j+\theta_j)}=e^{\mathrm{i}t\lambda_j}\zeta_j$$

for each j. Invoking Theorem 4.1.3, we conclude that PST occurs from $\mathbf{x}$ to $\mathbf{y}$ relative to M at time τ with phase factor γ and $|\Phi_{\mathbf{x}}|=r$. □

4.7 Constructions

In this section, we present constructions of pure states that admit PST.

Corollary 4.7.1. *Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *if and only if it occurs from* $\overline{\mathbf{y}}$ *to* $\overline{\mathbf{x}}$ *at the same time and the same phase factor.*

Proof. As $U(t)^{-1} = \overline{U(\tau)}$, we get $U(\tau)\mathbf{x} = \gamma\mathbf{y} \iff \overline{U(\tau)}\overline{\mathbf{x}} = \overline{\gamma\mathbf{y}} \iff U(\tau)\overline{\mathbf{y}} = \gamma\overline{\mathbf{x}}$. Alternatively, conjugating the equations in conditions 1 and 2 of Theorem 4.1.3 yields the desired result. □

Theorem 4.7.2. *Let* $\ell \geq 2$. *If perfect state transfer occurs from* $\mathbf{x}_j$ *to* $\mathbf{y}_j$ *for all* $j \in \{1 \dots, \ell\}$ *at the same time* τ *with phase factor* γ, *then for all* $(\alpha_1, \dots, \alpha_\ell) \in \mathbb{C}^\ell \backslash \{\mathbf{0}\}$, *perfect state transfer occurs from* $\sum_{j=1}^{\ell} \alpha_j \mathbf{x}_j$ *to* $\sum_{j=1}^{\ell} \alpha_j \mathbf{y}_j$ *at time* τ *with phase factor* γ.

Proof. By assumption, $U(\tau)\mathbf{x}_j = \gamma\mathbf{y}_j$ for each $j \in \{1, \dots, \ell\}$. Therefore,

$$U(\tau)\left(\sum_{j=1}^{\ell} \alpha_j \mathbf{x}_j\right) = \sum_{j=1}^{\ell} \alpha_j U(\tau)\mathbf{x}_j = \gamma \sum_{j=1}^{\ell} \alpha_j \mathbf{y}_j$$

from which our result follows. □

Our next result is straightforward from (3.6.2).

Theorem 4.7.3. *For* $j \in \{1, 2\}$, *let* $\mathbf{x}_j, \mathbf{y}_j \in \mathbb{C}^{n_j}$ *such that* $\mathbf{x}_1$ *and* $\mathbf{y}_1$ *are linearly independent. Perfect state transfer occurs from* $\mathbf{x}_1 \otimes \mathbf{x}_2$ *to* $\mathbf{y}_1 \otimes \mathbf{y}_2$ *at time* τ *relative to the Hamiltonian* $M_1 \otimes I_{n_2} + I_{n_1} \otimes M_2$ *if and only if either*

1. $\mathbf{x}_2$ *and* $\mathbf{y}_2$ *are linearly independent, perfect state transfer occurs from* $\mathbf{x}_1$ *to* $\mathbf{y}_1$ *relative to* M_1, *and from* $\mathbf{x}_2$ *to* $\mathbf{y}_2$ *relative to* M_2, *both at time* τ; *or*

2. $\mathbf{x}_2$ *and* $\mathbf{y}_2$ *are linearly dependent,* $\mathbf{x}_2$ *and* $\mathbf{y}_2$ *are periodic relative to* M_2 *at time* τ, *and perfect state transfer occurs from* $\mathbf{x}_1$ *to* $\mathbf{y}_1$ *relative to* M_1 *at time* τ.

If the Hamiltonian in Theorem 4.7.3 is replaced by $\alpha D + A$, then we get a result for Cartesian products of graphs. Next, we have the following result applies to direct products of graphs when the Hamiltonian is replaced by A.

Theorem 4.7.4. *Let* $m \geq 2$, $\mathbf{x} \in \mathbb{C}^{n_1}$ *and for* $j \in \{1, 2\}$, *let* $\mathbf{y}_j \in \mathbb{C}^{n_2}$. *Let* $\mathbf{y}_1$ *and* $\mathbf{y}_2$ *be* m*-strongly cospectral pure states and suppose perfect state transfer occurs from* $\mathbf{y}_1$ *to* $\mathbf{y}_2$ *relative to* M_2 *with minimum PST time* τ *and phase factor* γ *that is* *a primitive pth root of unity. If p divides m and each $\lambda \in \Phi_{\mathbf{x}}$ is an integer such that $\lambda \equiv 1 \pmod{m}$, then perfect state transfer occurs from $\mathbf{x} \otimes \mathbf{y}_1$ to $\mathbf{x} \otimes \mathbf{y}_2$ relative to $M_1 \otimes M_2$ at time τ and phase factor γ.*

Proof. By assumption, $U_{M_2}(\tau)\mathbf{y}_1 = \gamma \mathbf{y}_2$ for some unit complex number γ. As $\mathbf{y}_1$ and $\mathbf{y}_2$ are m-strongly cospectral, invoking Corollary 4.2.4 yields $U_{M_2}(\ell\tau)\mathbf{y}_1 = \gamma^{\ell}\mathbf{y}_2$ for any integer $\ell \equiv 1 \pmod{m}$. Because p divides m, we have $\gamma^{\ell} = \gamma$. Moreover, since each $\lambda \in \Phi_{\mathbf{x}}$ is an integer such that $\lambda \equiv 1 \pmod{m}$, (3.6.7) gives us

$$U_{M_1 \otimes M_2}(\tau)(\mathbf{x} \otimes \mathbf{y}_1) = \sum_{\lambda \in \Phi_{\mathbf{x}}} E_{\lambda}\mathbf{x} \otimes U_{M_2}(\lambda\tau)\mathbf{y}_1 = \sum_{\lambda \in \Phi_{\mathbf{x}}} E_{\lambda}\mathbf{x} \otimes \gamma^{\lambda}\mathbf{y}_2 = \gamma(\mathbf{x} \otimes \mathbf{y}_2).$$

Equivalently, PST occurs from $\mathbf{x} \otimes \mathbf{y}_1$ to $\mathbf{x} \otimes \mathbf{y}_2$ relative to $M_1 \otimes M_2$ at time τ and phase factor γ. $\square$

Lastly, we have a result about joins.

Theorem 4.7.5. *Let $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}, \mathbf{y} = \begin{bmatrix} \mathbf{y}_1 \\ \mathbf{y}_2 \end{bmatrix} \in \mathbb{C}^{n_1+n_2}$ and $\mathbf{x}_1, \mathbf{y}_1 \in \mathbb{C}^{n_1}$ with $\mathbf{1}^T\mathbf{x}_1 = \mathbf{1}^T\mathbf{x}_2 = 0$. If X and Y are connected graphs, then the following hold.*

1. *Let $\mathbf{x}_1 \neq 0$ and $\mathbf{x}_2 = 0$. Then perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $X \vee Y$ relative to $M \in \{A, L\}$ if and only if perfect state transfer occurs from $\mathbf{x}_1$ to $\mathbf{y}_1$ in X at the same time.*

2. *Let $\mathbf{x}_1, \mathbf{x}_2 \neq 0$. Relative to A, perfect state transfer occurs from $\mathbf{x}_1$ to $\mathbf{y}_1$ in X, and from $\mathbf{x}_2$ to $\mathbf{y}_2$ in Y both at time τ if and only if perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $X \vee Y$ at time τ with the same phase factor. Relative to L, perfect state transfer occurs from $\mathbf{x}_1$ to $\mathbf{y}_1$ in X, and from $\mathbf{x}_2$ to $\mathbf{y}_2$ in Y both at time τ with phase factors γ_1 and γ_2 satisfying $\gamma_1 e^{\mathrm{i}\tau n_2} = \gamma_2 e^{\mathrm{i}\tau n_2}$ if and only if perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $X \vee Y$ at time τ.*

Proof. If $\mathbf{1}^T\mathbf{x}_1 = \mathbf{1}^T\mathbf{x}_2 = 0$ and X, Y are connected, then (3.6.11) and (3.6.15) respectively gives us

$$U_L(t)\mathbf{x} = \begin{bmatrix} e^{\mathrm{i}tn_2}U_{L(X_1)}(t)\mathbf{x}_1 \\ e^{\mathrm{i}tn_1}U_{L(X_2)}(t)\mathbf{x}_2 \end{bmatrix} \quad \text{and} \quad U_A(t)\mathbf{x} = \begin{bmatrix} U_{A(X_1)}(t)\mathbf{x}_1 \\ U_{A(X_2)}(t)\mathbf{x}_2 \end{bmatrix}.$$

From this, the above Theorem is immediate. $\square$

5

PST between m-strongly cospectral states

As we have seen in the previous chapter, m-strongly cospectral pure states are special because perfect state transfer on such quantum states not only requires periodicity for the pure states involved (see Theorem 4.2.3), but it also satisfies a weak symmetry property (see Theorem 4.3.3), a ‘cyclic’ property (see Theorem 4.4.2(2)) and a non-monogamy property when $m \geq 3$ (see Corollary 4.4.3).

In this chapter, we further examine perfect state transfer on m-strongly cospectral pure states. We provide a number-theoretic characterisation for perfect state transfer on such pure states, and characterise all paths and cycles that admit perfect state transfer on m-strongly cospectral pure states relative to A and L. We also determine the forms of all pure states $\mathbf{y}$ that admit perfect state transfer from an arbitrary vector $\mathbf{x}$ in complete graphs and complete bipartite graphs relative to A and L. Last but not the least, we utilise results on the spread of graphs to prove that among all n-vertex simple unweighted graphs, the least minimum PST time on m-strongly cospectral pure states relative to the Laplacian is attained by any join graph, while relative to the adjacency, it is attained by the join of an empty graph and a complete graph of appropriate sizes.

5.1 Characterisations

We start with the main result in this chapter.

Theorem 5.1.1. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ *with* $\Phi_{\mathbf{x}} = \{\lambda_1, \ldots, \lambda_r\}$, *where* $r \geq 3$. *Let* $m \geq 2$ *and suppose* $\mathbf{x}$ *and* $\mathbf{y}$ *are* m*-strongly cospectral with* $E_j\mathbf{x} = e^{\mathrm{i}2\pi\ell_j/m}E_j\mathbf{y}$ *for each* j, *where* $\ell_j \in \mathbb{Z}_m$ *and* $\gcd(\ell_j, m) = 1$ *for some* j*. Then perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *if and only if both conditions below hold.*

1. *For each* $j \geq 2$, $\frac{\lambda_1-\lambda_j}{\lambda_1-\lambda_2} = \frac{p_j}{q_j}$*, where* $p_j, q_j \in \mathbb{Z}$ *and* $\gcd(p_j, q_j) = 1$*.*
2. *For each* $j \geq 2$, $\frac{qp_j}{q_j} \equiv \ell_j - \ell_1$ *(mod* m*), where* $q = \operatorname{lcm}(q_2, q_3, \ldots, q_r)$ *and* $p_2 = q_2 = 1$*. In particular,* $q \equiv \ell_2 - \ell_1$ *(mod* m*).*

In addition, if $q \equiv 0$*, then* $\ell_1 = \ell_j$ *if and only if* $\nu_m(q) > \nu_m(q_j)$*. Meanwhile, if* $q \not\equiv 0$ *(mod* m*), then* $\ell_1 = \ell_j$ *if and only if* $p_j \equiv 0$ *(mod* m*). Furthermore, the minimum PST time is* $\tau = \frac{\rho}{m}$*, where* ρ *is given in Theorem 3.7.8(2).*

Proof. Let $E_j\mathbf{x} = e^{\mathrm{i}2\pi\ell_j/m}E_j\mathbf{y}$ for each j, where $\ell_j \in \mathbb{Z}_m$ and $\gcd(\ell_j, m) = 1$ for some j. PST occurs from $\mathbf{x}$ to $\mathbf{y}$ with minimum PST time τ if and only if condition 2 of Theorem 4.1.3(2) holds. Equivalently, $e^{\mathrm{i}\tau(\lambda_1-\lambda_j)} = e^{\mathrm{i}2\pi(\ell_j-\ell_1)/m}$. That is,

$$\tau(\lambda_1 - \lambda_j) = 2\pi(\ell_j - \ell_1)/m + 2\pi s_j \tag{5.1.1}$$

for some integer $s_j \geq 0$. Without loss of generality, suppose $\lambda_1 > \lambda_2$. By the last statement in Theorem 4.4.2, $\mathbf{x}$ and $\mathbf{y}$ are periodic with a minimum period $\rho = m\tau$, where $\rho = \frac{2\pi q}{\lambda_1-\lambda_2}$, where $q = \operatorname{lcm}(q_3, \ldots, q_r)$, and p_j, q_j are integers satisfying $\frac{\lambda_1-\lambda_j}{\lambda_1-\lambda_2} = \frac{p_j}{q_j}$ and $\gcd(p_j, q_j) = 1$. This proves 1. Since $\tau = \frac{2\pi q}{m(\lambda_1-\lambda_2)}$, (5.1.1) gives us $\frac{qp_j}{q_j} \equiv \ell_j - \ell_1$ (mod m) for each $j \geq 2$. In particular, since $p_2 = q_2 = 1$, we get $q \equiv \ell_2 - \ell_1$ (mod m). This proves 2. The converse is immediate.

Now, suppose $q \equiv 0$ (mod m). Since each q_j divides q and $\gcd(p_j, q_j) = 1$, it follows that either (i) $q_j \equiv 0$ (mod m) and $p_j \not\equiv 0$ (mod m), or (ii) $q_j \not\equiv 0$ (mod m). For case (i), it must be that $\ell_j - \ell_1 \neq 0$ (mod m) whenever $\nu_m(q) > \nu_m(q_j)$ while $\ell_j - \ell_1 \neq 0$ (mod m) whenever $\nu_m(q) = \nu_m(q_j)$. For case (ii), it must be that $\ell_j - \ell_1 \neq 0$ (mod m). It follows that $\ell_1 = \ell_j$ (mod m) if and only if $\nu_m(q) > \nu_m(q_j)$. On the other hand, if $q \not\equiv 0$ (mod m), then each $q_j \not\equiv 0$ (mod m). Hence, $\ell_j - \ell_1 \neq 0$ (mod m) if and only if $p_j \equiv 0$ (mod m). □

If we restrict the elements of $\Phi_{\mathbf{x}}$ in Theorem 5.1.1 to be algebraic integers, then we obtain the following result.

Corollary 5.1.2. *With the assumptions in Theorem 5.1.1, suppose in addition that* $\ell_1 = \ell_2$ *in* $\mathbb{Z}_m$ *and* $\Phi_{\mathbf{x}}$ *is a set of real algebraic integers closed under taking algebraic conjugates. Then perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *if and only if both conditions below hold.*

1. *For each $j \geq 1$, $\lambda_j = \frac{1}{2}(a + b_j\sqrt{\Delta})$, where $\Delta \geq 1$ is a square-free integer and a, b_j are integers, and each λ_j is an integer whenever $\Delta = 1$.*

2. *For each $j \geq 3$, we have*

$$\frac{\lambda_1 - \lambda_j}{g\sqrt{\Delta}} \equiv \ell_j - \ell_1 \ (mod\ m)$$

   In particular, $\ell_1 = \ell_j$ if and only if $\nu_m(\frac{\lambda_1-\lambda_j}{\sqrt{\Delta}}) > \nu_m(g)$, where g is given by $g = \gcd(\frac{\lambda_1-\lambda_2}{\sqrt{\Delta}}, \dots, \frac{\lambda_1-\lambda_r}{\sqrt{\Delta}})$.

Further, the minimum PST time is given by $\tau = \frac{2\pi}{mg\sqrt{\Delta}}$.

Proof. Combining Theorem 5.1.1(1) and Theorem 2.3.5 yields 1. Using the form of λ_j's in 1, we get $q = \operatorname{lcm}(q_2, \dots, q_r) = \operatorname{lcm}(\frac{b_1-b_2}{g_2}, \dots, \frac{b_1-b_2}{g_r}) = \frac{b_1-b_2}{g} = \frac{\lambda_1-\lambda_2}{g\sqrt{\Delta}}$ and $q_j = \frac{b_1-b_2}{g_j} = \frac{\lambda_1-\lambda_2}{g_j\sqrt{\Delta}}$, where $g_j = \gcd(\frac{\lambda_1-\lambda_2}{\sqrt{\Delta}}, \frac{\lambda_1-\lambda_j}{\sqrt{\Delta}})$. Thus, we have

$$\frac{qp_j}{q_j} = \frac{\left(\frac{b_1-b_2}{g}\right)\left(\frac{b_1-b_j}{g_j}\right)}{\frac{b_1-b_2}{g_j}} = \frac{b_1 - b_j}{g} = \frac{\lambda_1 - \lambda_j}{g\sqrt{\Delta}}.$$

Hence, $\frac{qp_j}{q_j} \equiv \ell_j - \ell_1 \pmod{m}$ if and only if $\frac{\lambda_1-\lambda_j}{g\sqrt{\Delta}} \equiv \ell_j - \ell_1 \pmod{m}$. And so it follows that $\ell_1 = \ell_j$ if and only if $\nu_m(\frac{\lambda_1-\lambda_j}{\sqrt{\Delta}}) > \nu_2(g)$. □

Remark 5.1.3. Suppose $m < r$ (equivalently, there are more spectral idempotents than the elements of $\mathbb{Z}_m$). By the Pigeonhole Principle, there is at least one $\ell \in \mathbb{Z}_m$ such that $E_j\mathbf{x} = e^{i2\pi\ell/m}E_j\mathbf{y}$ and $E_k\mathbf{x} = e^{i2\pi\ell/m}E_k\mathbf{y}$ for at least two indices j, k. In this case, we may reorder the eigenvalues in Theorem 5.1.1 such that $j = 1$ and $k = 2$, in which case $\ell_1 = \ell_2$. Consequently, Corollary 5.1.2 applies whenever $m < r$.

5.2 Complete graphs

Here, we characterise PST in simple unweighted complete graphs K_n relative to the adjacency matrix $M = A$. Since complete graphs are regular, our results for this family also apply to the Hamiltonian $\alpha D + A$ for all $\alpha \in \mathbb{R}$.

Theorem 5.2.1. *Perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in K_n at time τ relative to $\alpha D + A$ if and only if $\mathbf{x} \notin \operatorname{span}\{\mathbf{1}\}$, $\mathbf{x}$ is not orthogonal to $\mathbf{1}$, $\gamma = e^{-i\tau}$ and*

$$\mathbf{y} = \mathbf{x} + \left(\frac{(e^{i\tau n} - 1)\mathbf{1}^T\mathbf{x}}{n}\right)\mathbf{1}. \tag{5.2.1}$$

Additionally, if $\mathbf{x}, \mathbf{y}$ *are* m*-strongly cospectral, then the minimum PST time is* $\frac{2\pi}{mn}$*.*

Proof. If $\mathbf{x} \in \operatorname{span}\{\mathbf{1}\}$ or $\mathbf{x}$ is orthogonal to $\mathbf{1}$, then $\mathbf{x}$ is fixed. Otherwise, (3.1.6) yields $e^{\mathrm{i}t}U_A(t)\mathbf{x} = \mathbf{x} + \left(\frac{(e^{\mathrm{i}tn}-1)\mathbf{1}^T\mathbf{x}}{n}\right)\mathbf{1}$. By Theorem 3.7.8(1), K_n is periodic with $\rho = \frac{2\pi}{n}$, and so applying the last statement in Theorem 4.4.2 completes the proof. □

From Theorem 5.2.1, any vector $\mathbf{x} \in \mathbb{C}^n$ such that $\mathbf{x} \notin \operatorname{span}\{\mathbf{1}\}$ and $\mathbf{x}$ is not orthogonal to $\mathbf{1}$ admits PST in K_n at any time τ, and for a fixed choice of τ, the vector $\mathbf{y}$ to which $\mathbf{x}$ admits PST to is given in (5.2.1). This illustrates that in general, there is no direct connection between the minimum PST time and the minimum period, unless we impose the additional assumption that $\mathbf{x}$ and $\mathbf{y}$ are m-strongly cospectral, in which case $\rho = m\tau$ by the last statement in Theorem 4.4.2.

5.3 Complete bipartite graphs

Next, we characterise PST in simple unweighted complete bipartite graphs $K_{a,b}$ relative to the adjacency matrix $M \in \{A, L\}$, starting with the case $M = A$.

Theorem 5.3.1. *Let* $\mathbf{x} = \begin{bmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{bmatrix}, \mathbf{y} \in \mathbb{C}^{a+b}$*, where* $\mathbf{x}_1 \in \mathbb{C}^a$*. Let* $\mathbf{z}$ *and* $\mathbf{v}^{\pm} = \begin{bmatrix}\sqrt{b}\mathbf{1}_a\\ \pm\sqrt{a}\mathbf{1}_b\end{bmatrix}$ *be eigenvectors for* $A(K_{a,b})$ *associated with 0 and* $\pm\sqrt{ab}$ *respectively. Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *in* $K_{a,b}$ *at time* τ *and phase factor* γ *relative to* A *if and only if* $|\Phi_{\mathbf{x}}| \geq 2$*,* $\gamma = 1$ *and*

$$\mathbf{y} = \mathbf{x} + \begin{bmatrix}\left((\mathbf{1}^T\mathbf{x}_1)(\operatorname{Re}(e^{\mathrm{i}\tau\sqrt{ab}}) - 1)\frac{1}{a} + (\mathbf{1}^T\mathbf{x}_2)\mathrm{i}\operatorname{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\frac{1}{\sqrt{ab}}\right)\mathbf{1}\\ \left((\mathbf{1}^T\mathbf{x}_1)\mathrm{i}\operatorname{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\frac{1}{\sqrt{ab}} + (\mathbf{1}^T\mathbf{x}_2)(\operatorname{Re}(e^{\mathrm{i}\tau\sqrt{ab}}) - 1)\frac{1}{b}\right)\mathbf{1}\end{bmatrix}. \tag{5.3.1}$$

Additionally, if $\mathbf{x}, \mathbf{y}$ *are* m*-strongly cospectral, then the minimum PST time is* $\frac{2\pi}{m\sqrt{ab}}$*.*

Proof. Since $K_{a,b} = O_a \vee O_b$, (3.6.14) yields the spectral decomposition for $A(K_{a,b})$:

$$U_A(t) = \begin{bmatrix}I_a - \frac{1}{a}J & 0\\ 0 & I_b - \frac{1}{b}J\end{bmatrix} + \frac{e^{\mathrm{i}t\sqrt{ab}}}{2ab}\begin{bmatrix}bJ & \sqrt{ab}J\\ \sqrt{ab}J & aJ\end{bmatrix} + \frac{e^{-\mathrm{i}t\sqrt{ab}}}{2ab}\begin{bmatrix}bJ & -\sqrt{ab}J\\ -\sqrt{ab}J & aJ\end{bmatrix}.$$

The condition that $\mathbf{x} \in \operatorname{span}\{\mathbf{v}^+, \mathbf{v}^-, \mathbf{z}\}$ and $\mathbf{x} \notin \operatorname{span}\mathcal{W}$ for any two-subset $\mathcal{W}$ of $\{\mathbf{v}^+, \mathbf{v}^-, \mathbf{z}\}$ guarantees that $|\Phi_{\mathbf{x}}(A)| \geq 3$. Simplifying $\mathbf{y} = U_A(\tau)\mathbf{x}$ yields the form of $\mathbf{y}$ in the above theorem. Applying the last statement in Theorem 4.4.2 completes the proof. □

Relative to L, (3.6.10) gives us the transition matrix for $K_{a,b}$:

$$U_L(t) = \frac{1}{n}J + \frac{e^{\mathrm{i}tn}}{abn}\begin{bmatrix} b^2J & -abJ \\ -abJ & a^2J \end{bmatrix} + e^{\mathrm{i}tb}\begin{bmatrix} I_a - \frac{1}{a}J & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} + e^{\mathrm{i}ta}\begin{bmatrix} \mathbf{0} & \mathbf{0} \\ \mathbf{0} & I_b - \frac{1}{b}J \end{bmatrix},$$

where $n = a + b$. Using the same argument in the proof of Theorem 5.3.1 yields the following result.

Theorem 5.3.2. *Let* $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}, \mathbf{y} \in \mathbb{C}^{a+b}$, *where* $\mathbf{x}_1 \in \mathbb{C}^a$. *Let* $\mathbf{u}$, $\mathbf{v}$ *and* $\mathbf{w}$ *be eigenvectors for* $L(K_{a,b})$ *associated with* a, b *and* $n = a + b$ *respectively. Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *in* $K_{a,b}$ *at time* τ *and phase factor* γ *relative to* L *if and only if* $|\Phi_{\mathbf{x}}| \geq 2$, $\gamma = 1$ *and*

$$\mathbf{y} = \begin{bmatrix} e^{\mathrm{i}\tau b}\mathbf{x}_1 + \left(\frac{\mathbf{1}^T\mathbf{x}_1}{an}(a + be^{\mathrm{i}\tau n} - ne^{\mathrm{i}\tau b}) + \frac{\mathbf{1}^T\mathbf{x}_2}{n}(1 - e^{\mathrm{i}\tau n})\right)\mathbf{1} \\ e^{\mathrm{i}\tau a}\mathbf{x}_2 + \left(\frac{\mathbf{1}^T\mathbf{x}_2}{bn}(b + ae^{\mathrm{i}\tau n} - ne^{\mathrm{i}\tau a}) + \frac{\mathbf{1}^T\mathbf{x}_1}{n}(1 - e^{\mathrm{i}\tau n})\right)\mathbf{1} \end{bmatrix}. \tag{5.3.2}$$

Additionally, if $\mathbf{x}, \mathbf{y}$ *are* m*-strongly cospectral, then the minimum PST time is* $\frac{\pi}{m \gcd(a,b)}$.

Remark 5.3.3. Let $|\Phi_{\mathbf{x}}(A)| \geq 3$. Relative to A, perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $K_{a,b}$ at time τ and phase factor γ if and only $\mathbf{y}$ has the form given in (5.3.1) and $\mathbf{x} \in \operatorname{span}\{\mathbf{v}^+, \mathbf{v}^-, \mathbf{z}\}$, $\mathbf{x} \notin \operatorname{span}\mathcal{W}$ for any two-subset $\mathcal{W}$ of $\{\mathbf{v}^+, \mathbf{v}^-, \mathbf{z}\}$. Meanwhile, relative to A, perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $K_{a,b}$ at time τ and phase factor γ if and only $\mathbf{y}$ has the form given in (5.3.2) and $\mathbf{x} \in \operatorname{span}\{\mathbf{1}, \mathbf{u}, \mathbf{v}, \mathbf{w}\}$, $\mathbf{x} \notin \operatorname{span}\mathcal{W}$ for any two-subset $\mathcal{W}$ of $\{\mathbf{1}, \mathbf{u}, \mathbf{v}, \mathbf{w}\}$.

Example 5.3.4. Let $\mathbf{x} = \begin{bmatrix} \mathbf{1}_a \\ \mathbf{0} \end{bmatrix}, \mathbf{y} \in \mathbb{C}^{a+b}$. Note that $\mathbf{x}$ is the characteristic vector of the partite set of $K_{a,b}$ with size a. By Theorem 5.3.1, we have PST in $K_{a,b}$ from $\mathbf{x}$ to $\mathbf{y}$ at time τ relative to A if and only if

$$\mathbf{y} = \begin{bmatrix} \mathbf{1}_a + (\operatorname{Re}(e^{\mathrm{i}\tau\sqrt{ab}}) - 1)\mathbf{1}_a \\ (\mathrm{i}\operatorname{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\frac{\sqrt{a}}{\sqrt{b}})\mathbf{1}_b \end{bmatrix}.$$

Thus, if $\tau = \frac{\pi}{2\sqrt{ab}}$, then $\mathbf{y} = \begin{bmatrix} \mathbf{0} \\ -\frac{\sqrt{a}}{\sqrt{b}}\mathbf{1}_b \end{bmatrix}$. Now, by Theorem 5.3.2, we have PST in $K_{a,b}$ from $\mathbf{x}$ to $\mathbf{y}$ at time τ relative to L if and only if

$$\mathbf{y} = \begin{bmatrix} \frac{1}{n}\left(a + be^{\mathrm{i}\tau n}\right)\mathbf{1}_a \\ \left(\frac{a}{n}(1 - e^{\mathrm{i}\tau n})\right)\mathbf{1}_b \end{bmatrix}.$$

Figure 5.1: Let S_1 and S_2 be the set of vertices coloured blue and pink, respectively. Up to a normalization factor, PST occurs from $\mathbf{e}_{S_1}$ to $\mathbf{e}_{S_2}$ in $K_{2,3}$ relative to A but not L (left), and PST occurs from $\mathbf{e}_{S_1}$ to $\mathbf{e}_{S_2}$ in $K_{3,3}$ relative to A and L (right).

Thus, if $\tau = \frac{\pi}{n}$, then $\mathbf{y} = \begin{bmatrix} \frac{1}{n}(a-b)\,\mathbf{1}_a \\ \frac{2a}{n}\mathbf{1}_b \end{bmatrix}$. In particular, $\mathbf{y} = \begin{bmatrix} \mathbf{0} \\ \mathbf{1}_b \end{bmatrix}$ whenever $a = b$. This example illustrates that any bipartite graph has perfect state transfer from the characteristic vector of one partite set to another (scaled) relative to A, while this is only possible relative to L when the partite sets have equal sizes. See Figure 5.1.

5.4 Cycles

For cycles, we adopt the convention that $V(C_n) = \mathbb{Z}_n$ and vertices j, k are adjacent whenever $|k - j| \equiv 1 \pmod{n}$. The eigenvalues and eigenvectors of C_n are well-known, see [16, Section 1.4.3]. For our purposes, we provide normalised eigenvectors for C_n in the following lemma.

Lemma 5.4.1. *The eigenvalues of $A(C_n)$ are $\theta_j = 2\cos(2j\pi/n)$, where $0 \le j \le \lfloor \frac{n}{2} \rfloor$. An associated eigenvector for $\theta_0 = 2$ is $\mathbf{v}_0 = \frac{1}{\sqrt{n}}\mathbf{1}$, while an associated eigenvector for $\theta_{\frac{n}{2}} = -2$ whenever n is even is $\mathbf{v}_{\frac{n}{2}} = \frac{1}{\sqrt{n}}[1, -1, 1, -1, \dots, 1, -1]^T$. For $1 \le j < \frac{n}{2}$, we have the following associated eigenvectors for λ_j:*

$$\mathbf{v}_j = \sqrt{\frac{2}{n}} \left[\ 1, \ \cos\left(\frac{2j\pi}{n}\right), \ \cos\left(\frac{4j\pi}{n}\right), \ \cdots, \ \cos\left(\frac{2j(n-1)\pi}{n}\right) \ \right]^T$$

and

$$\mathbf{v}_{n-j} = \sqrt{\frac{2}{n}} \left[\ 0, \ \sin\left(\frac{2j\pi}{n}\right), \ \sin\left(\frac{4j\pi}{n}\right), \ \cdots, \ \sin\left(\frac{2j(n-1)\pi}{n}\right) \ \right]^T.$$

Moreover, $\{\mathbf{v}_0, \dots, \mathbf{v}_{n-1}\}$ is an orthonormal basis for $\mathbb{R}^n$.

We are now ready to characterise m-strongly cospectral pure states that admit PST in cycles. Since Corollary 4.5.1 takes care of the case $|\Phi_{\mathbf{x}}| = 2$, we only focus on the case when $|\Phi_{\mathbf{x}}| \geq 3$. Moreover, since cycles are regular, our results for this family relative to A also apply to the Hamiltonian $\alpha D + A$ for all $\alpha \in \mathbb{R}$.

Theorem 5.4.2. *Let $m \geq 2$, $n \geq 3$ and $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. Suppose $\mathbf{x}$ and $\mathbf{y}$ are m-strongly cospectral, $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(A)$ is closed under taking algebraic conjugates and $|\Phi_{\mathbf{x}}| \geq 3$. Then C_n admits perfect state transfer from $\mathbf{x}$ to $\mathbf{y}$ relative to $\alpha D + A$ if and only if one of the following conditions hold.*

1. *$n = 2k$, $\mathbf{x} = a\mathbf{v}_0 + b(\alpha_1 \mathbf{v}_{\frac{n}{6}} + \alpha_2 \mathbf{v}_{\frac{5n}{6}}) + c(\beta_1 \mathbf{v}_{\frac{n}{4}} + \beta_2 \mathbf{v}_{\frac{3n}{4}}) + d(\gamma_1 \mathbf{v}_{\frac{n}{3}} + \gamma_2 \mathbf{v}_{\frac{2n}{3}}) + e\mathbf{v}_{\frac{n}{2}}$ and $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m} a\mathbf{v}_0 + e^{-\mathrm{i}2\pi\ell_2/m} b(\alpha_1 \mathbf{v}_{\frac{n}{6}} + \alpha_2 \mathbf{v}_{\frac{5n}{6}}) + e^{-\mathrm{i}2\pi\ell_3/m} c(\beta_1 \mathbf{v}_{\frac{n}{4}} + \beta_2 \mathbf{v}_{\frac{3n}{4}}) + e^{-\mathrm{i}2\pi\ell_4/m} d(\gamma_1 \mathbf{v}_{\frac{n}{3}} + \gamma_2 \mathbf{v}_{\frac{2n}{3}}) + e^{-\mathrm{i}2\pi\ell_5/m} e\mathbf{v}_{\frac{n}{2}}$, all conditions below hold mod m*

   $$\ell_2 - \ell_1 \equiv \frac{1}{g}, \quad \ell_3 - \ell_1 \equiv \frac{2}{g}, \quad \ell_4 - \ell_1 \equiv \frac{3}{g} \quad \textit{and} \quad \ell_5 - \ell_1 \equiv \frac{4}{g},$$

   and one of the conditions below hold.

   (a) *If $b \neq 0$ or $d \neq 0$, and $c = 0$, then $k \equiv 0$ (mod 3) and $g = 1$. In this case, $\Phi_{\mathbf{x}} \subseteq \{\pm 1, \pm 2\}$.*

   (b) *If $b \neq 0$ or $d \neq 0$, and $c \neq 0$, then $k \equiv 0$ (mod 6) and $g = 1$. In this case, $0 \in \Phi_{\mathbf{x}}$, $\Phi_{\mathbf{x}} \subseteq \{0, \pm 1, \pm 2\}$ and $\Phi_{\mathbf{x}} \neq \{0, \pm 2\}$.*

   (c) *If $b = d = 0$, and $c \neq 0$, then $k \equiv 0$ (mod 2) and and $g = 2$. In this case $\Phi_{\mathbf{x}} = \{0, \pm 2\}$.*

2. *$n = 12k$, $\mathbf{x} = a(\alpha_1 \mathbf{v}_{3k} + \alpha_2 \mathbf{v}_{9k}) + b(\beta_1 \mathbf{v}_k + \beta_2 \mathbf{v}_{11k}) + c(\gamma_1 \mathbf{v}_{5k} + \gamma_2 \mathbf{v}_{7k})$ and $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m} a(\alpha_1 \mathbf{v}_{3k} + \alpha_2 \mathbf{v}_{9k}) + e^{-\mathrm{i}2\pi\ell_2/m} b(\beta_1 \mathbf{v}_k + \beta_2 \mathbf{v}_{11k}) + e^{-\mathrm{i}2\pi\ell_3/m}(\gamma_1 \mathbf{v}_{5k} + \gamma_2 \mathbf{v}_{7k})$ and the following conditions hold mod m:*

   $$\ell_2 - \ell_1 \equiv m - 1 \quad \textit{and} \quad \ell_3 - \ell_1 \equiv 1. \tag{5.4.1}$$

   In this case, $\Phi_{\mathbf{x}} = \{0, \pm\sqrt{3}\}$.

3. *$n = 8k$, $\mathbf{x} = a(\alpha_1 \mathbf{v}_{2k} + \alpha_2 \mathbf{v}_{6k}) + b(\beta_1 \mathbf{v}_k + \beta_2 \mathbf{v}_{7k}) + c(\gamma_1 \mathbf{v}_{3k} + \gamma_2 \mathbf{v}_{5k})$ and $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m} a(\alpha_1 \mathbf{v}_{2k} + \alpha_2 \mathbf{v}_{6k}) + e^{-\mathrm{i}2\pi\ell_2/m} b(\beta_1 \mathbf{v}_k + \beta_2 \mathbf{v}_{7k}) + e^{-\mathrm{i}2\pi\ell_3/m} c(\gamma_1 \mathbf{v}_{3k} + \gamma_2 \mathbf{v}_{5k})$ and both conditions in (5.4.1) hold mod m. In this case $\Phi_{\mathbf{x}}(M) = \{0, \pm\sqrt{2}\}$.*

In all cases above, each $\ell_j \in \mathbb{Z}_m$ and $\gcd(\ell_j, m) = 1$ for at least one j. Moreover, $a, b, c, d, e \in \mathbb{C}$ are such that $|a|^2 + |b|^2 + |c|^2 = \|\mathbf{x}\|^2$ in 2-3 with $a, b, c \neq 0$, and $|a|^2 + |b|^2 + |c|^2 + |d|^2 + |e|^2 = \|\mathbf{x}\|^2$ otherwise. Furthermore, $(\alpha_1, \alpha_2), (\beta_1, \beta_2), (\gamma_1, \gamma_2) \in \mathbb{C}^2 \backslash \{(0,0)\}$ such that $|\alpha_1|^2 + |\alpha_2|^2 = |\beta_1|^2 + |\beta_2|^2 = |\gamma_1|^2 + |\gamma_2|^2 = 1$. The minimum PST times in 1(a), 1(b), 1(c), 2 and 3 are $\frac{2\pi}{m}$, $\frac{2\pi}{m}$, $\frac{\pi}{m}$, $\frac{2\pi}{m\sqrt{3}}$ and $\frac{2\pi}{m\sqrt{2}}$, respectively.

Proof. Let $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(A)$ be closed under taking algebraic conjugates and assume $|\Phi_{\mathbf{x}}(A)| \geq 3$. Since A is an integer matrix, $\Phi_{\mathbf{x}}$ consists of real algebraic integers. Thus, we may invoke Corollary 5.1.2. Assume $\mathbf{x}$ and $\mathbf{y}$ are m-strongly cospectral pure states, and PST occurs from $\mathbf{x}$ to $\mathbf{y}$. By Corollary 5.1.2(1), the eigenvalues in $\Phi_{\mathbf{x}}$ are either all integers, or all quadratic integers. Thus, by Corollary 3.7.18, the elements in $\Phi_{\mathbf{x}}$ differ by at least one. Since $|\theta_j| \leq 2$ by Lemma 5.4.1, we get $|\Phi_{\mathbf{x}}| \leq 5$. We have two cases.

Case 1. Let $\Phi_{\mathbf{x}} \subseteq \mathbb{Z}$ so that $\Phi_{\mathbf{x}} \subseteq \{0, \pm 1, \pm 2\}$. By Proposition 3.3.2, we may express

$$\mathbf{x} = a\mathbf{v}_0 + b\mathbf{u} + c\mathbf{w} + d\mathbf{z} + e\mathbf{v}_{\frac{n}{2}},$$

where $a, b, c, d, e \in \mathbb{C}$ and $\mathbf{u}, \mathbf{w}, \mathbf{z}$ are eigenvectors associated with $\theta_{\frac{n}{6}} = 1$, $\theta_{\frac{n}{4}} = 0$, $\theta_{\frac{n}{3}} = -1$, respectively. The latter implies that we may write

$$\mathbf{u} = \alpha_1 \mathbf{v}_{\frac{n}{6}} + \alpha_2 \mathbf{v}_{\frac{5n}{6}}, \quad \mathbf{w} = \beta_1 \mathbf{v}_{\frac{n}{4}} + \beta_2 \mathbf{v}_{\frac{3n}{4}}, \quad \text{and} \quad \mathbf{z} = \gamma_1 \mathbf{v}_{\frac{n}{3}} + \gamma_2 \mathbf{v}_{\frac{2n}{3}},$$

where $(\alpha_1, \alpha_2), (\beta_1, \beta_2), (\gamma_1, \gamma_2) \in \mathbb{C}^2 \backslash \{(0, 0)\}$. As $|\Phi_{\mathbf{x}}| \geq 3$, $\Phi_{\mathbf{x}}$ contains one of $0, 1, -2$, and hence n must be even. Write $n = 2m$ for some integer m. Since $\mathbf{x}, \mathbf{y}$ are m-strongly cospectral, Theorem 3.5.12 allows us to write

$$\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m} a\mathbf{v}_0 + e^{-\mathrm{i}2\pi\ell_2/m} b\mathbf{u} + e^{-\mathrm{i}2\pi\ell_3/m} c\mathbf{w} + e^{-\mathrm{i}2\pi\ell_4/m} d\mathbf{z} + e^{-\mathrm{i}2\pi\ell_5/m} e\mathbf{v}_{\frac{n}{2}},$$

where each $\ell_j \in \mathbb{Z}_m$ and $\gcd(\ell_j, m) = 1$ for at least one j. Invoking Corollary 5.1.2(2) with $\lambda_1 = 2$, $\lambda_2 = 1$, $\lambda_3 = 0$ $\lambda_4 = -1$ and $\lambda_5 = -2$, we get PST from $\mathbf{x}$ to $\mathbf{y}$ if and only if $\ell_2 - \ell_1 \equiv \frac{1}{g}$, $\ell_3 - \ell_1 \equiv \frac{2}{g}$, $\ell_4 - \ell_1 \equiv \frac{3}{g}$ and $\ell_5 - \ell_1 \equiv \frac{4}{g} \pmod{m}$. In particular, we have two subcases.

- Let $b \neq 0$ or $d \neq 0$. Then $\frac{n}{6}$ or $\frac{n}{3}$ is an integer. If $c = 0$, then we get $m \equiv 0 \pmod{3}$ and $\Phi_{\mathbf{x}} \subseteq \{\pm 2, \pm 1\}$. This proves 1(a). If $c \neq 0$, then we also have that $\frac{n}{4}$ is an integer, and so $m \equiv 0 \pmod{6}$. In this case, $0 \in \Phi_{\mathbf{x}}$, $\Phi_{\mathbf{x}} \subseteq \{\pm 2, 0, \pm 1\}$, and $\Phi_{\mathbf{x}} \neq \{0, \pm 2\}$. This proves 1(b). In both cases, $g = 1$.
- Let $b = 0$ and $d = 0$. As $|\Phi_{\mathbf{x}}| = 3$, we have $0 \in \Phi_{\mathbf{x}}$. Thus, $c \neq 0$ which implies that $n \equiv 0 \pmod{4}$. In this case, $\Phi_{\mathbf{x}} = \{0, \pm 2\}$ and $g = 2$. This proves 1(c).

Case 2. Let $\Phi_{\mathbf{x}}(A) \subseteq \{\frac{a}{2}, \frac{1}{2}(a \pm b_1\sqrt{\Delta}), \frac{1}{2}(a \pm b_2\sqrt{\Delta})\}$, where a, b_1, b_2, Δ are integers such that $b_1 > b_2 > 0$ and $\Delta > 1$ is square-free. Note that $\frac{a}{2}$ is an integer as it is a root of a polynomial with integer coefficients. Since $|\frac{a}{2}| \leq 2$, we get $a \in \{0, \pm 2, \pm 4\}$. If $a = 2$, then $|\frac{1}{2}(2 \pm b_j\sqrt{\Delta})| \leq 2$ implies that $b_j = 1$ and $\Delta \in \{2, 3\}$. However,

$\frac{1}{2}(2 \pm \sqrt{\Delta})$ are not quadratic integers whenever $\Delta \in \{2,3\}$. Thus, $a \neq 2$ and similarly, $a \neq -2$. Now, if $a = 0$, then $|\frac{1}{2}b_j\sqrt{\Delta}| \leq 2$, where $\frac{1}{2}b_j$ is an integer, and so we get that $b_j = 2$ and $\Delta \in \{2,3\}$. Since $b_1 \neq b_2$, the case $|\Phi_{\mathbf{x}}(A)| \in \{4,5\}$ does not happen. Thus, $|\Phi_{\mathbf{x}}(A)| = 3$ and $\Delta \in \{2,3\}$. We have the following subcases.

- Let $\Delta = 3$ so that $\Phi_{\mathbf{x}} = \{0, \pm\sqrt{3}\}$. By Lemma 5.4.1, $\{0, \pm\sqrt{3}\} \subseteq \operatorname{spec}(A(C_n))$ if and only if $n = 12m$ and $j \in \{\frac{n}{4}, \frac{n}{12}, \frac{5n}{12}\}$. Thus, $\mathbf{x} = a\mathbf{z} + b\mathbf{u} + c\mathbf{w}$, where $\mathbf{z} = \alpha_1\mathbf{v}_{\frac{n}{4}} + \alpha_2\mathbf{v}_{\frac{3n}{4}}$, $\mathbf{u} = \beta_1\mathbf{v}_{\frac{n}{12}} + \beta_2\mathbf{v}_{\frac{11n}{12}}$ and $\mathbf{w} = \gamma_1\mathbf{v}_{\frac{5n}{12}} + \gamma_2\mathbf{v}_{\frac{7n}{12}}$.
- Let $\Delta = 2$, so that $\Phi_{\mathbf{x}} = \{0, \pm\sqrt{2}\}$. A similar argument yields $n = 8m$ and $\mathbf{x} = a\mathbf{z} + b\mathbf{u} + c\mathbf{w}$, where $\mathbf{z} = \alpha_1\mathbf{v}_{\frac{n}{4}} + \alpha_2\mathbf{v}_{\frac{3n}{4}}$, $\mathbf{u} = \beta_1\mathbf{v}_{\frac{n}{8}} + \beta_2\mathbf{v}_{\frac{7n}{8}}$ and $\mathbf{w} = \gamma_1\mathbf{v}_{\frac{3n}{8}} + \gamma_2\mathbf{v}_{\frac{5n}{8}}$.

Using the same argument in Case 1 yields 2-3. The Pythagorean relations involving a, b, c, d, e and $(\alpha_1, \alpha_2), (\beta_1, \beta_2), (\gamma_1, \gamma_2)$ follow from the fact that $\{\mathbf{v}_j\}$ is an orthonormal basis for $\mathbb{R}^n$. The minimum PST times are immediate from Corollary 5.1.2. ☐

Remark 5.4.3. Fix $m \geq 2$. For each $n \geq 3$, let τ_n be the least minimum PST time in C_n amongst all m-strongly cospectral pure states relative to A. If n is even, then we have $\tau_n = \frac{\pi}{2m}$, which is attained by $\mathbf{x} = a\mathbf{v}_0 + b\mathbf{v}_{\frac{n}{2}}$ and $\mathbf{y} = a\mathbf{v}_0 + e^{\mathrm{i}2\pi\ell/m}b\mathbf{v}_{\frac{n}{2}}$, where $\ell \in \mathbb{Z}_m$ such that $\gcd(\ell, m) = 1$. In this case, $\Phi_{\mathbf{x}} = \{\pm 2\}$ and τ_n is independent of n. On the other hand, if n is odd, then we have $\tau_n = \frac{\pi}{m(1+\cos(\frac{\pi}{n}))}$, which is attained by $\mathbf{x} = a\mathbf{v}_0 + b\mathbf{v}_{\frac{n-1}{2}}$ and $\mathbf{y} = a\mathbf{v}_0 + e^{\mathrm{i}2\pi\ell/m}b\mathbf{v}_{\frac{n-1}{2}}$, where $\ell \in \mathbb{Z}_m$ such that $\gcd(\ell, m) = 1$. In this case, $\Phi_{\mathbf{x}} = \{2, -2\cos(\frac{\pi}{n})\}$ and $\tau_n \to \frac{\pi}{2m}$ as $n \to \infty$.

From Theorem 5.4.2, the following is immediate.

Corollary 5.4.4. *If n is not divisible by 4 or 6, then perfect state transfer does not occur in C_n between m-strongly cospectral pure states relative to $\alpha D + A$. In particular, perfect state transfer does not occur in C_n between real pure states.*

The following example illustrates Theorem 5.4.2.

Example 5.4.5. Let $m \geq 2$ and $n = 2k$ for some $k \equiv 0 \pmod 4$. Invoking Theorem 5.4.2(1(c)), the vectors

$$\mathbf{x} = a\mathbf{v}_0 + c(\beta_1\mathbf{v}_{\frac{n}{4}} + \beta_2\mathbf{v}_{\frac{3n}{4}}) + e\mathbf{v}_{\frac{n}{2}} \tag{5.4.2}$$

and

$$\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{v}_0 + e^{-\mathrm{i}2\pi\ell_3/m}c(\beta_1\mathbf{v}_{\frac{n}{4}} + \beta_2\mathbf{v}_{\frac{3n}{4}}) + e^{-\mathrm{i}2\pi\ell_5/m}e\mathbf{v}_{\frac{n}{2}} \tag{5.4.3}$$

admit PST in C_n if and only if the following hold mod m:

$$\ell_3 - \ell_1 \equiv 1, \quad \text{and} \quad \ell_5 - \ell_1 \equiv 2. \tag{5.4.4}$$

In this case, $\Phi_{\mathbf{x}} = \{0, \pm 2\}$, the minimum PST time is $\frac{\pi}{m}$, $a^2 + c^2 + e^2 = \|\mathbf{x}\|^2$ and $\beta_1^2 + \beta_2^2 = 1$. Additionally, if $\ell_1 = 0$ and $a = e = \frac{1}{\sqrt{2}}c = \frac{\sqrt{n}}{4}$, then the following hold from (5.4.2), (5.4.3) and (5.4.4).

1. Let $m = 2$, $\ell_3 = 1$ and $\ell_5 = 0$. Then $\mathbf{x}$ and $\mathbf{y}$ are real pure states admitting PST at time $\frac{\pi}{2}$.
   (a) If $(\beta_1, \beta_2) = (1, 0)$, then $\mathbf{x} = a(\mathbf{v}_0 + \sqrt{2}\mathbf{v}_{\frac{n}{4}} + \mathbf{v}_{\frac{n}{2}}) = \sum_{j=0}^{\frac{n}{4}-1} \mathbf{e}_{4j}$ and $\mathbf{y} = a(\mathbf{v}_0 - \sqrt{2}\mathbf{v}_{\frac{n}{4}} + \mathbf{v}_{\frac{n}{2}}) = \sum_{j=0}^{\frac{n}{4}-1} \mathbf{e}_{4j+2}$. In particular, if $n = 8$, then $\mathbf{x} = \mathbf{e}_0 + \mathbf{e}_4$ and $\mathbf{y} = \mathbf{e}_2 + \mathbf{e}_6$, while if $n = 12$, then $\mathbf{x} = \mathbf{e}_0 + \mathbf{e}_4 + \mathbf{e}_6$ and $\mathbf{y} = \mathbf{e}_2 + \mathbf{e}_6 + \mathbf{e}_{10}$.
   (b) If $(\beta_1, \beta_2) = (0, 1)$, then $\mathbf{x} = a(\mathbf{v}_0 + \sqrt{2}\mathbf{v}_{\frac{3n}{4}} + \mathbf{v}_{\frac{n}{2}}) = [1, 1, 1, -1, \dots, 1, 1, 1, -1]$ and $\mathbf{y} = a(\mathbf{v}_0 - \sqrt{2}\mathbf{v}_{\frac{3n}{4}} + \mathbf{v}_{\frac{n}{2}}) = [1, -1, 1, 1, \dots, 1, -1, 1, 1]$. In particular, if $n = 8$, then $\mathbf{x} = [1, 1, 1, -1, 1, 1, 1, -1]$ and $\mathbf{y} = [1, -1, 1, 1, 1, -1, 1, 1]$.
2. Let $m = 4$, $\ell_3 = 1$ and $\ell_5 = 2$. Then $\mathbf{x}$ and $\mathbf{y}$ admit PST at time $\frac{\pi}{4}$, where $\mathbf{x}$ is a real pure state and $\mathbf{y}$ is a nonreal pure state. In particular, the following hold.
   (a) If $(\beta_1, \beta_2) = (1, 0)$, then $\mathbf{x} = a(\mathbf{v}_0 + \sqrt{2}\mathbf{v}_{\frac{n}{4}} + \mathbf{v}_{\frac{n}{2}}) = \sum_{j=0}^{\frac{n}{4}-1} \mathbf{e}_{4j}$ and $\mathbf{y} = a(\mathbf{v}_0 - \mathrm{i}\sqrt{2}\mathbf{v}_{\frac{n}{4}} - \mathbf{v}_{\frac{n}{2}}) = \frac{1}{2}[-\mathrm{i}, 1, \mathrm{i}, 1, \dots, -\mathrm{i}, 1, \mathrm{i}, 1]$. In particular, if $n = 8$, then $\mathbf{x} = \mathbf{e}_0 + \mathbf{e}_4$ and $\mathbf{y} = \frac{1}{2}[-\mathrm{i}, 1, \mathrm{i}, 1, -\mathrm{i}, 1, \mathrm{i}, 1]$.
   (b) If $(\beta_1, \beta_2) = (0, 1)$, then $\mathbf{x} = a(\mathbf{v}_0 + \sqrt{2}\mathbf{v}_{\frac{3n}{4}} + \mathbf{v}_{\frac{n}{2}}) = [1, 1, 1, -1, \dots, 1, 1, 1, -1]$ and $\mathbf{y} = a(\mathbf{v}_0 - \mathrm{i}\sqrt{2}\mathbf{v}_{\frac{3n}{4}} - \mathbf{v}_{\frac{n}{2}}) = \sum_{j \text{ odd}} \mathbf{e}_j + \mathrm{i} \sum_{j \text{ odd}} \mathbf{e}_j$. In particular, if $n = 8$, then we obtain $\mathbf{x} = [1, 1, 1, -1, 1, 1, 1, -1]$ and $\mathbf{y} = (1 - \mathrm{i})[0, 1, 0, \mathrm{i}, 0, 1, 0, \mathrm{i}]$.

5.5 Paths

For paths, we adopt the convention that the vertices of P_n are labelled so that vertices j, k are adjacent whenever $|k - j| = 1$. We start with the adjacency matrix. The adjacency eigenvalues and eigenvectors of P_n are well-known, see [16, Section 1.4.4]. Again for our purposes, we provide normalised eigenvectors for $A(P_n)$ below.

Lemma 5.5.1. *For each* $j \in \{1, \ldots, n\}$*, an eigenvector associated with an eigenvalue* $\mu_j = 2\cos\left(\frac{j\pi}{n+1}\right)$ *of* $A(P_n)$ *is*

$$\mathbf{z}_j = \sqrt{\frac{2}{n+1}} \left[\; \sin\left(\frac{j\pi}{n+1}\right), \; \sin\left(\frac{2j\pi}{n+1}\right), \; \ldots, \; \sin\left(\frac{nj\pi}{n+1}\right) \; \right]^T .$$

Moreover, $\{\mathbf{z}_1, \ldots, \mathbf{z}_n\}$ *forms an orthonormal basis for* $\mathbb{R}^n$*.*

We now characterise PST on pure states in paths relative to A. Again, since Corollary 4.5.1 takes care of the case $|\Phi_{\mathbf{x}}| = 2$, we only focus on the case $|\Phi_{\mathbf{x}}| \geq 3$.

Theorem 5.5.2. *Let* $m \geq 2$*,* $n \geq 3$ *and* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$*. Suppose* $\mathbf{x}$ *and* $\mathbf{y}$ *are* m*-strongly cospectral,* $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(A)$ *is closed under taking algebraic conjugates and* $|\Phi_{\mathbf{x}}| \geq 3$*. Then* P_n *admits perfect state transfer from* $\mathbf{x}$ *to* $\mathbf{y}$ *relative to* A *if and only if one of the following conditions hold.*

1. $n+1 = 6k$*, and either*
   - *(a)* $\mathbf{x} = a\mathbf{z}_{3k} + b\mathbf{z}_{2k} + c\mathbf{z}_{4k}$*,* $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{z}_{3k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{z}_{2k} + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{z}_{4k}$ *and the conditions in (5.4.1) hold mod* m*. In this case,* $\Phi_{\mathbf{x}} = \{0, \pm 1\}$*.*
   - *(b)* $\mathbf{x} = a\mathbf{z}_{3k} + b\mathbf{z}_{k} + c\mathbf{z}_{5k}$*,* $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{z}_{3k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{z}_{k} + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{z}_{5k}$ *and the conditions in (5.4.1) hold mod* m*. In this case,* $\Phi_{\mathbf{x}} = \{0, \pm\sqrt{3}\}$*.*
2. $n+1 = 4k$*,* $\mathbf{x} = a\mathbf{z}_{2k} + b\mathbf{z}_{k} + c\mathbf{z}_{3k}$*,* $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{z}_{2k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{z}_{k} + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{z}_{3k}$ *and the conditions in (5.4.1) hold mod* m*. In this case,* $\Phi_{\mathbf{x}} = \{0, \pm\sqrt{2}\}$*.*

In all cases above, each $\ell_j \in \mathbb{Z}_m$ *and* $\gcd(\ell_j, m) = 1$ *for at least one* j*. Moreover,* $a, b, c \in \mathbb{C}\backslash\{0\}$ *are such that* $|a|^2 + |b|^2 + |c|^2 = \|\mathbf{x}\|^2$*. Moreover, the minimum PST times in 1(a), 1(b) and 2 are* $\frac{2\pi}{m}$*,* $\frac{2\pi}{m\sqrt{3}}$ *and* $\frac{2\pi}{m\sqrt{2}}$*, respectively.*

Proof. Let $|\Phi_{\mathbf{x}}| \geq 3$ and $\Phi_{\mathbf{x}}$ be closed under algebraic conjugates. As $|\mu_j| < 2$, Corollary 3.7.18 yields $|\Phi_{\mathbf{x}}(A)| = 3$. By Lemma 3.7.3, we get two cases. If $\Phi_{\mathbf{x}}(A) \subseteq \mathbb{Z}$, then using the same argument as Case 1 of the proof of Theorem 5.4.2 to show 1(a). If $\Phi_{\mathbf{x}}(A) = \{\frac{a}{2}, \frac{1}{2}(a \pm b\sqrt{\Delta})\}$, then one may use the argument in Case 2 to obtain 1(b) and (2). □

The following is immediate from Theorem 5.5.2.

Corollary 5.5.3. *If* $n+1$ *is not divisible by 4 or 6, then perfect state transfer does not occur in* P_n *between* m*-strongly cospectral pure states relative to* A*. In particular, perfect state transfer does not occur in* P_n *between real pure states relative to* A*.*

We now illustrate Theorem 5.5.2.

Example 5.5.4. Let $m \geq 2$ and $n+1 = 4k$. Invoking Theorem 5.5.2(2), the vectors

$$\mathbf{x} = a\mathbf{z}_{2k} + b\mathbf{z}_k + c\mathbf{z}_{3k} \tag{5.5.1}$$

and

$$\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{z}_{2k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{z}_k + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{z}_{3k} \tag{5.5.2}$$

admit PST in P_n relative to A if and only if the following hold mod m:

$$\ell_2 - \ell_1 \equiv m-1, \quad \text{and} \quad \ell_3 - \ell_1 \equiv 1. \tag{5.5.3}$$

In this case, $\Phi_{\mathbf{x}} = \{0, \pm\sqrt{2}\}$, the minimum PST time is $\frac{2\pi}{m\sqrt{2}}$ and $a^2+b^2+c^2 = \|\mathbf{x}\|^2$. Additionally, if $\ell_1 = 0$, then (5.5.1), (5.5.2) and (5.5.3) yield the following.

1. Let $m = 2$, $\ell_2 = \ell_3 = 1$, and $a = \sqrt{2}b = \sqrt{2}c = \frac{\sqrt{n+1}}{2\sqrt{2}}$. Then $\mathbf{x}$ and $\mathbf{y}$ are real pure states admitting PST at time $\frac{\pi}{\sqrt{2}}$, where

$$\mathbf{x} = a\left(\mathbf{z}_{2k} + \frac{1}{\sqrt{2}}(\mathbf{z}_k + \mathbf{z}_{3k})\right) = \sum_{j=0}^{\lfloor \frac{k-1}{2} \rfloor} \mathbf{e}_{8j+1} - \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} \mathbf{e}_{8j-1}$$

   and

$$\mathbf{y} = a(\mathbf{z}_{2k} - \frac{1}{\sqrt{2}}(\mathbf{z}_k + \mathbf{z}_{3k})) = \sum_{j=1}^{\lfloor \frac{k}{2} \rfloor} \mathbf{e}_{8j-3} - \sum_{j=0}^{\lfloor \frac{k-1}{2} \rfloor} \mathbf{e}_{8j+3},$$

   where the second summand in the first equation and the first summand in the second equation are absent when $k = 1$. In particular, the following hold.

   (a) If $k = 1$, then we have PST between $\mathbf{e}_1$ and $\mathbf{e}_3$ in P_3.

   (b) If $k = 2$, then we have PST between $\mathbf{e}_1 - \mathbf{e}_7$ and $\mathbf{e}_3 - \mathbf{e}_5$ in P_7.

   (c) If $k = 3$, then PST occurs between $\mathbf{e}_1 - \mathbf{e}_7 + \mathbf{e}_9$ and $\mathbf{e}_3 - \mathbf{e}_5 + \mathbf{e}_{11}$ in P_{11}.

2. Let $m = 4$, $\ell_2 = 3$, $\ell_3 = 1$, and $a = 2b = 2c = \frac{\sqrt{n+1}}{\sqrt{2}}$. Then $\mathbf{x}$ and $\mathbf{y}$ admit PST at time $\frac{\pi}{2\sqrt{2}}$, where

$$\begin{aligned}\mathbf{x} &= a\left(\mathbf{z}_{2k} + \frac{1}{2}(\mathbf{z}_k + \mathbf{z}_{3k})\right) \\ &= \sum_{j=1}^{\frac{n+1}{4}} \left[\mathbf{e}_{4j-3}\left(1 + \frac{\sqrt{2}}{2}(-1)^{j-1}\right) + \mathbf{e}_{4j-1}\left(-1 + \frac{\sqrt{2}}{2}(-1)^{j-1}\right)\right]\end{aligned}$$

and

$$\mathbf{y} = a\left(\mathbf{z}_{2k} + \mathrm{i}\frac{1}{2}(\mathbf{z}_k - \mathbf{z}_{3k})\right) = \sum_{j=1}^{\frac{n+1}{4}} (\mathbf{e}_{4j-3} - \mathbf{e}_{4j-1}) + \mathrm{i}\sum_{j=1}^{\frac{n+1}{4}} \mathbf{e}_{4j-2}.$$

In this case, $\mathbf{x}$ is a real pure state and $\mathbf{y}$ is a nonreal pure state. In particular, the following hold.

(a) If $k = 1$, then we have PST from $[1 + \frac{\sqrt{2}}{2}, 0, -1 + \frac{\sqrt{2}}{2}]$ to $[1, \mathrm{i}, -1]$ in P_3.

(b) If $k = 2$, then we have PST from $[1 + \frac{\sqrt{2}}{2}, 0, 1 - \frac{\sqrt{2}}{2}, +\frac{\sqrt{2}}{2}, 0, -1 - \frac{\sqrt{2}}{2}]$ to $[1, \mathrm{i}, -1, 0, 1, \mathrm{i}, -1]$ in P_7.

For the Laplacian case, the eigenvalues and eigenvectors of P_n are well-known, see [16, Section 1.4.4]. We provide normalised eigenvectors for $L(P_n)$ below.

Lemma 5.5.5. *For $j \in \{1, \dots n-1\}$, an eigenvector associated with an eigenvalue $\theta_j = 2\left(1 - \cos\left(\frac{j\pi}{n}\right)\right)$ of $L(P_n)$ is*

$$\mathbf{w}_j = \sqrt{\frac{2}{n}}\left[\ \cos\left(\frac{j\pi}{2n}\right),\ \cos\left(\frac{3j\pi}{2n}\right),\ \cos\left(\frac{5j\pi}{2n}\right),\ \dots,\ \cos\left(\frac{(2n-1)j\pi}{2n}\right)\ \right]^T$$

while an eigenvector associated with $\theta_0 = 0$ is $\mathbf{w}_0 = \frac{1}{\sqrt{n}}\mathbf{1}$. Moreover, $\{\mathbf{w}_0, \dots, \mathbf{w}_{n-1}\}$ is an orthonormal basis for $\mathbb{R}^n$.

The same argument in the proof of Theorem 5.5.2 yields an analogous result for the Laplacian case.

Theorem 5.5.6. *Let $m \geq 2$, $n \geq 3$ and $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$. Suppose $\mathbf{x}$ and $\mathbf{y}$ are m-strongly cospectral, $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(A)$ is closed under taking algebraic conjugates and $|\Phi_{\mathbf{x}}| \geq 3$. Then P_n admits perfect state transfer from $\mathbf{x}$ to $\mathbf{y}$ relative to L if and only if one of the following conditions hold.*

1. *$n = 3k$, $\mathbf{x} = a\mathbf{w}_{2k} + b\mathbf{w}_{\frac{3k}{2}} + c\mathbf{w}_k + d\mathbf{w}_0$, $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{w}_{2k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{w}_{\frac{3k}{2}} + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{w}_k + e^{-\mathrm{i}2\pi\ell_4/m}d\mathbf{w}_0$, k is even whenever $b \neq 0$ and the following conditions hold mod m*

   $$\ell_2 - \ell_1 \equiv 1, \quad \ell_3 - \ell_1 \equiv 2, \quad \textit{and} \quad \ell_4 - \ell_1 \equiv 3.$$

   In this case, $\Phi_{\mathbf{x}} = \{3, 2, 1, 0\}$ if $b \neq 0$ and $\Phi_{\mathbf{x}} = \{3, 1, 0\}$ otherwise.

2. *$n = 6k$, $\mathbf{x} = a\mathbf{w}_{3k} + b\mathbf{w}_{5k} + c\mathbf{w}_k$, $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{w}_{3k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{w}_{5k} + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{w}_k$ and the conditions in (5.4.1) hold mod m. Here, $\Phi_{\mathbf{x}} = \{2, 2 \pm \sqrt{3}\}$.*

3. *$n = 4k$, $\mathbf{x} = a\mathbf{w}_{2k} + b\mathbf{w}_{3k} + c\mathbf{w}_k$, $\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m}a\mathbf{w}_{2k} + e^{-\mathrm{i}2\pi\ell_2/m}b\mathbf{w}_{3k} + e^{-\mathrm{i}2\pi\ell_3/m}c\mathbf{w}_k$ and the conditions in (5.4.1) hold mod m. Here, $\Phi_{\mathbf{x}} = \{2, 2 \pm \sqrt{2}\}$.*

In all cases, $a, b, c, d \in \mathbb{C}$ *are such that* $|a|^2 + |b|^2 + |c|^2 + |d|^2 = \|\mathbf{x}\|^2$ *in (1) and* $|a|^2 + |b|^2 + |c|^2 = \|\mathbf{x}\|^2$ *otherwise. Moreover, the minimum PST times in 1, 2 and 3 are* $\frac{2\pi}{m}$, $\frac{2\pi}{m\sqrt{3}}$ *and* $\frac{2\pi}{m\sqrt{2}}$, *respectively.*

Remark 5.5.7. If the coefficients $a, b, c, d, e \in \mathbb{C}$ of the vector $\mathbf{x}$ in Theorems 5.4.2, 5.5.2 and 5.5.6 are chosen such that $a^2 = e^{\mathrm{i}2\pi\ell_1/m}$, $b^2 = e^{\mathrm{i}2\pi\ell_2/m}$, $c^2 = e^{\mathrm{i}2\pi\ell_3/m}$, $d^2 = e^{\mathrm{i}2\pi\ell_4/m}$, and $e^2 = e^{\mathrm{i}2\pi\ell_5/m}$, then we obtain a characterisation PST on vectors $\mathbf{x}$ and its conjugate $\overline{\mathbf{x}}$ which are m-strongly cospectral.

From Theorem 5.5.6, the following is straightforward.

Corollary 5.5.8. *If n is not divisible by 3 or 4, then perfect state transfer does not occur in P_n between m-strongly cospectral pure states relative to L. In particular, perfect state transfer does not occur in P_n between real pure states relative to L.*

The next example illustrates Theorem 5.5.6.

Example 5.5.9. Let $m \geq 2$ and suppose $n = 3k$. Invoking Theorem 5.5.6(1), the vectors

$$\mathbf{x} = a\mathbf{w}_{2k} + c\mathbf{w}_k + d\mathbf{w}_0 \tag{5.5.4}$$

and

$$\mathbf{y} = e^{-\mathrm{i}2\pi\ell_1/m} a\mathbf{w}_{2k} + e^{-\mathrm{i}2\pi\ell_3/m} c\mathbf{w}_k + e^{-\mathrm{i}2\pi\ell_4/m} d\mathbf{w}_0 \tag{5.5.5}$$

admit PST in P_n relative to L if and only if the following hold mod m:

$$\ell_3 - \ell_1 \equiv 2, \quad \text{and} \quad \ell_4 - \ell_1 \equiv 3. \tag{5.5.6}$$

In this case, $\Phi_{\mathbf{x}} = \{3, 1, 0\}$, the minimum PST time is $\frac{2\pi}{m}$ and $a^2 + c^2 + d^2 = \|\mathbf{x}\|^2$. Additionally, if $\ell_1 = 0$, then (5.5.4), (5.5.5) and (5.5.6) yield the following.

1. Let $m = 2$, $\ell_3 = 0$, $\ell_4 = 1$ and $a = \frac{c}{\sqrt{3}} = \frac{d}{\sqrt{2}} = \frac{\sqrt{n}}{3\sqrt{2}}$. Then $\mathbf{x}$ and $\mathbf{y}$ are real pure states admitting PST at time π, where

$$\mathbf{x} = a\left(\mathbf{w}_{2k} + \sqrt{3}\mathbf{w}_k + \sqrt{2}\mathbf{w}_0\right) = \sum_{\substack{j=1 \\ j \text{ odd}}}^{\frac{n}{3}} \mathbf{e}_{3j-2} + \sum_{\substack{j=1 \\ j \text{ even}}}^{\frac{n}{3}} \mathbf{e}_{3j}$$

and

$$\begin{aligned}\mathbf{y} &= a\left(\mathbf{w}_{2k} + \sqrt{3}\mathbf{w}_k - \sqrt{2}\mathbf{w}_0\right) \\ &= \frac{1}{3}\left(\sum_{\substack{j=1 \\ j \text{ odd}}}^{\frac{n}{3}} (\mathbf{e}_{3j-2} - 2\mathbf{e}_{3j-1} - 2\mathbf{e}_{3j}) - \sum_{\substack{j=1 \\ j \text{ even}}}^{\frac{n}{3}} (2\mathbf{e}_{3j-2} + 2\mathbf{e}_{3j-1} - \mathbf{e}_{3j})\right)\end{aligned}$$

In particular, the following hold.

(a) If $k=1$, then we have PST between $\mathbf{e}_1$ and $\frac{1}{3}[1,-2,-2]$ in P_3.

(b) If $k=2$, then PST between $\mathbf{e}_1+\mathbf{e}_6$ and $\frac{1}{3}[1,-2,-2,-2,-2,1]$ in P_6.

2. Let $m=4$, $\ell_3=2$, $\ell_4=3$, and $a=\frac{c}{\sqrt{3}}=\frac{d}{\sqrt{2}}=\frac{\sqrt{n}}{3\sqrt{2}}$. Then $\mathbf{x}$ and $\mathbf{y}$ admit PST at time $\frac{\pi}{2}$, where $\mathbf{x}$ has the same form as above and

$$\mathbf{y}=a(\mathbf{w}_{2k}-\sqrt{3}\mathbf{w}_k+\mathrm{i}\sqrt{2}\mathbf{w}_0)=\frac{1}{3}\sum_{\substack{j=1\\ j\text{ odd}}}^{\frac{n}{3}}(\mathrm{i}-1)(\mathbf{e}_{3j-2}+\mathbf{e}_{3j-1})+(\mathrm{i}+2)\mathbf{e}_{3j})$$
$$+\frac{1}{3}\sum_{\substack{j=1\\ j\text{ odd}}}^{\frac{n}{3}}(\mathrm{i}-1)(\mathbf{e}_{3j-1}+\mathbf{e}_{3j})+(\mathrm{i}+2)\mathbf{e}_{3j-2}).$$

In this case, $\mathbf{x}$ is a real pure state and $\mathbf{y}$ is a nonreal pure state. In particular, the following hold.

(a) If $k=1$, then we have PST from $\mathbf{e}_1$ to $\frac{1}{3}[\mathrm{i}-1,\mathrm{i}-1,\mathrm{i}+2]$ in P_3.

(b) If $k=2$, then PST from $\mathbf{e}_1+\mathbf{e}_6$ to $\frac{1}{3}[\mathrm{i}-1,\mathrm{i}-1,\mathrm{i}+2,\mathrm{i}+2,\mathrm{i}-1,\mathrm{i}-1]$ in P_6.

We close the section with the following remark.

Remark 5.5.10. Fix $m\geq 2$. For each $n\geq 3$, let τ_n be the least minimum PST time in P_n amongst m-strongly cospectral pure states. We have $\tau_n=\frac{\pi}{2m\cos(\frac{\pi}{n+1})}$ relative to A, attained by $\mathbf{x}=a\mathbf{z}_1+b\mathbf{z}_n$ and $\mathbf{y}=a\mathbf{z}_1+e^{\mathrm{i}2\pi\ell/m}b\mathbf{z}_n$. In this case, $\Phi_{\mathbf{x}}=\{\pm 2\cos(\frac{\pi}{n+1})\}$. Meanwhile, we have $\tau_n=\frac{\pi}{m\left(1+\cos\left(\frac{\pi}{n}\right)\right)}$ relative to L, attained by $\mathbf{x}=a\mathbf{w}_0+b\mathbf{w}_{n-1}$ and $\mathbf{y}=a\mathbf{w}_0+e^{\mathrm{i}2\pi\ell/m}b\mathbf{w}_{n-1}$. In this case, $\Phi_{\mathbf{x}}=\{0,2(1-\cos(\frac{(n-1)\pi}{n}))\}$. In both cases, we must have $\ell\in\mathbb{Z}_m$ such that $\gcd(\ell,m)=1$ and $\tau_n\to\frac{\pi}{2m}$ as $n\to\infty$.

5.6 Minimising PST time

The following result determines the pure states $\mathbf{x}$ and graphs X such that the minimum period of $\mathbf{x}$ in X is the least amongst all unweighted connected n-vertex graphs.

Theorem 5.6.1. *Let $\mathbf{x}\in\mathbb{C}^n$ and $M\in\{A,L\}$. The following hold.*

1. *Amongst all connected unweighted n-vertex graphs, $\mathbf{x}$ attains the least minimum period in X relative to L if and only if $X=G_1\vee G_2$ with $|V(G_j)|=n_j$ for $j\in\{1,2\}$, $n=n_1+n_2$, and $\mathbf{x}\in\operatorname{span}\left\{\mathbf{1}_n,\begin{bmatrix}n_2\mathbf{1}_{n_1}\\-n_1\mathbf{1}_{n_2}\end{bmatrix}\right\}$.*

2. *There exists an integer* $N > 0$ *such that for all connected unweighted* n*-vertex graphs with* $n \geq N$*,* $\mathbf{x}$ *attains the least minimum period in* X *relative to* A *if and only if* $X = O_a \vee K_{n-a}$ *with* $a = \lceil \frac{n}{3} \rceil$*, and* $\mathbf{x} \in \operatorname{span}\left\{ \begin{bmatrix} -\lambda^- \mathbf{1}_a \\ a\mathbf{1}_{n-a} \end{bmatrix}, \begin{bmatrix} -\lambda^+ \mathbf{1}_a \\ a\mathbf{1}_{n-a} \end{bmatrix} \right\}$*, where* $\lambda^{\pm} = \frac{1}{2}(n-a-1 \pm \sqrt{(n-a-1)^2 + 4a(n-a)})$*.*

Moreover, for 1 and 2, we have $\rho = \frac{2\pi}{n}$ *and* $\rho = \frac{2\pi}{\sqrt{(n-a-1)^2+4a(n-a)}}$ $(\approx \frac{\pi\sqrt{3}}{n}$ *for large* $n)$*, respectively.*

Proof. Let λ_1 and λ_2 be the largest and smallest eigenvalues of M. We first prove 1. By assumption, 0 is a simple eigenvalue of $L(X)$ with eigenvector $\mathbf{1}_n$. Moreover, every eigenvalue λ of $L(X)$ satisfies $\lambda \leq n$ with equality if and only if X is a join graph. Thus, for any two eigenvalues λ_1 and λ_2 of $L(X)$, the Laplacian spread $\lambda_1 - \lambda_2$ is maximum if and only if $\lambda_1 = n$ and $\lambda_2 = 0$. Invoking Theorem 3.7.8(1), the least minimum period is attained if and only if $X = G_1 \vee G_2$ for some graphs G_j on n_j vertices, $j \in \{1, 2\}$ and $\Phi_{\mathbf{x}}(L) = \{0, n\}$, in which case $\rho = \frac{\pi}{n}$ and $\begin{bmatrix} n_2\mathbf{1}_{n_1} \\ -n_1\mathbf{1}_{n_2} \end{bmatrix}$ is the eigenvector associated with n. To prove 2, we use a result due to Breen, Riasanovsky, Tait and Urschel [15] states that there is an $N > 0$ such that if $n \geq N$, the maximum adjacency spread $\lambda_1 - \lambda_2$ over all connected n-vertex graphs is attained uniquely by the complete split graph $X = O_a \vee K_{n-a}$. In this case, we have $\lambda_1 = \lambda^+$, $\lambda_2 = \lambda^-$ and $\lambda^{\pm} = \frac{1}{2}(n-a-1 \pm \sqrt{(n-a-1)^2 + 4a(n-a)})$ so that $\lambda_1 - \lambda_2 = \sqrt{(n-a-1)^2 + 4a(n-a)}$ $(\approx \frac{2n}{\sqrt{3}}$ for large $n)$. The same argument used in the above case yields the desired conclusion. □

We are now ready to determine the forms of m-strongly cospectral pure states $\mathbf{x}, \mathbf{y}$ and the graphs X such that the minimum PST time from $\mathbf{x}$ to $\mathbf{y}$ in X is the least amongst all unweighted connected n-vertex graphs relative to A and L.

Corollary 5.6.2. *Fix* $m \geq 2$ *and let* $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ *be* m*-strongly cospectral.*

1. *Amongst all connected unweighted* n*-vertex graphs, the least minimum PST time from* $\mathbf{x}$ *to* $\mathbf{y}$ *relative to* L *is attained if and only if the conditions in Theorem 5.6.1(1) hold and*

$$\mathbf{y} = \frac{1}{n}(\mathbf{1}_n^T\mathbf{x})\mathbf{1}_n + e^{\mathrm{i}2\pi/m}\frac{1}{n_1n_2n}\left(\begin{bmatrix} n_2\mathbf{1}_{n_1} \\ -n_1\mathbf{1}_{n_2} \end{bmatrix}^T \mathbf{x}\right)\begin{bmatrix} n_2\mathbf{1}_{n_1} \\ -n_1\mathbf{1}_{n_2} \end{bmatrix}.$$

2. *There exists an integer* $N > 0$ *such that amongst all connected unweighted* n*-vertex graphs with* $n \geq N$*, the least minimum PST time from* $\mathbf{x}$ *to* $\mathbf{y}$ *relative*

to A is attained if and only if the conditions in Theorem 5.6.1(2) hold and $\mathbf{y}$ *has the form below, where* $D^{\pm} = \pm a(\lambda^{\pm})\sqrt{(n-a-1)^2 + 4a(n-a)}$.

$$\mathbf{y} = \frac{1}{D^-}\left(\begin{bmatrix} -\lambda^-\mathbf{1}_a \\ a\mathbf{1}_{n-a} \end{bmatrix}^T \mathbf{x}\right)\begin{bmatrix} -\lambda^-\mathbf{1}_a \\ a\mathbf{1}_{n-a} \end{bmatrix} + e^{\mathrm{i}2\pi/m}\frac{1}{D^+}\left(\begin{bmatrix} -\lambda^+\mathbf{1}_a \\ a\mathbf{1}_{n-a} \end{bmatrix}^T \mathbf{x}\right)\begin{bmatrix} -\lambda^+\mathbf{1}_a \\ a\mathbf{1}_{n-a} \end{bmatrix}.$$

The minimum PST time in 1 and 2 are $\frac{2\pi}{mn}$ *and* $\frac{2\pi}{m\sqrt{(n-a-1)^2+4a(n-a)}}$ ($\approx \frac{\pi\sqrt{3}}{mn}$ *for large* n*), respectively.*

Proof. This follows from Theorem 5.6.1, the fact that $|\Phi_{\mathbf{x}}(M)| = 2$, Theorem 3.7.8(1), and the last statement in Theorem 4.4.2. In particular, one may solve for $\mathbf{y}$ in 1 and 2 using (3.6.10) and (3.6.10) and noting that $\Phi_{\mathbf{x}}(L) = \{0, n\}$, $\Phi_{\mathbf{x}}(A) = \{\lambda^{\pm}\}$ and the minimum PST times are $\tau = \frac{2\pi}{mn}$ and $\tau = \frac{2\pi}{m\sqrt{(n-a-1)^2+4a(n-a)}}$ ($\approx \frac{\pi\sqrt{3}}{mn}$ for large n), respectively. □

We close this section with the following remarks.

Remark 5.6.3. As $n \to \infty$, the least minimum PST times in Corollary 5.6.2 both tend to 0, in contrast to the least minimum PST time for sparse graphs like paths which tend to $\frac{\pi}{2m}$ by Remark 5.5.10. Thus, the join graphs in Corollary 5.6.2 are desirable if a smaller minimum PST time is preferred.

6

Real state transfer

In this chapter, we focus on perfect state transfer on real pure states. We provide a characterisation of perfect state transfer on real pure states and show that such a characterisation coincides with that of PST on m-strongly cospectral pure states with $m = 2$. Our characterisation also recovers a well-known characterisation of perfect state transfer between vertex states due to Coutinho [32]. We also provide characterisations of weak and strong cospectrality on real pure states, which recovers the characterisations of cospectral and strongly cospectral vertices due to Godsil and Smith [56]. Moreover, we investigate the quantum state transfer properties of pure states with nonnegative entries. In particular, we show that periodicity of pure states with nonnegative rational entries is a rare phenomenon relative to a Hamiltonian with nonnegative entries. We also include a survey of results on unweighted graphs that admit perfect state transfer between real pure states.

Let $\mathbf{x} \neq \mathbf{0}$ be a real vector. Observe that for any time $t > 0$, there is perfect state transfer between $\mathbf{x}$ and $\gamma U(t)\mathbf{x}$ for some unit $\gamma \in \mathbb{C}$. But as $U(t)$ has complex entries, we are not guaranteed that $\gamma U(t)\mathbf{x}$ has real entries. Now, suppose $\gamma U(\tau)\mathbf{x}$ has real entries. If there is perfect state transfer between $\mathbf{x}$ and another vector $\mathbf{y} \in \mathbb{R}^n$, then Theorem 4.4.2 with $m = 2$ implies that $\mathbf{y} = \pm\gamma U(\tau)\mathbf{x}$. Without loss of generality suppose $\mathbf{y} = \gamma U(\tau)\mathbf{x}$. Additionally, if τ is the minimum PST time between $\mathbf{x}$ and $\mathbf{y}$, then Corollary 4.2.4 with $m = 2$ implies that every PST time is an odd multiple of τ. Hence, if $t = (2k+1)\tau$, then

$$\gamma U(t)\mathbf{x} = \gamma U(\tau)^{2k} U(\tau)\mathbf{x} = U(\tau)^{2k}\mathbf{y} = \gamma^{-2k}\mathbf{y}.$$

That is, $\mathbf{y} = \gamma^{2k+1} U(t)\mathbf{x}$. From this, we deduce that for every $\gamma \in \mathbb{C}$, there is at most one real vector in the set $\{\gamma U(t)\mathbf{x} : t > 0\}$ distinct from $\pm\mathbf{x}$. This demonstrates that the existence perfect state transfer between real pure states is a special occurrence, and therefore warrants an investigation.

This chapter is based closely on a joint work of the author with Dr. Stephen Kirkland and Dr. Chris Godsil [53]. The results presented in this chapter are the contributions of the author to this joint work.

6.1 Perfect state transfer

In this section, we survey results about perfect state transfer between real pure states that are immediate from the previous chapters.

If $\mathbf{x}$ and $\mathbf{y}$ are real vectors that are strongly cospectral, then they are 2-strongly cospectral. Applying Theorem 4.2.3 and Corollary 4.2.4, we recover a fundamental result about periods and PST times between real pure states, first established by Godsil in Lemmas 2.3 and 5.2 in [52].

Corollary 6.1.1. *Let* $\mathbf{x}$ *and* $\mathbf{y}$ *be real vectors. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *with minimum PST time* τ*, then the following hold.*

1. *Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *at any odd multiple of* τ*.*
2. $\mathbf{x}$ *and* $\mathbf{y}$ *are periodic any even multiple of* τ *and their minimum period is* 2τ*. That is, the minimum period is half the minimum PST time.*

The next result is immediate from Corollary 4.4.5 by taking $m = 2$.

Theorem 6.1.2. *Let* $\mathbf{x}, \mathbf{y}, \mathbf{z} \in \mathbb{R}^n$*. If perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$*, and from* $\mathbf{x}$ *to* $\mathbf{z}$*, then* $\mathbf{y} = \pm\mathbf{z}$*.*

Invoking Corollary 4.7.1 or Theorem 4.3.3 with $m = 2$ and $\zeta = \gamma^2$, we recover the symmetry property of PST between real pure states first observed by Godsil [52].

Corollary 6.1.3. *Let* $\mathbf{x}$ *and* $\mathbf{y}$ *be real vectors. Perfect state transfer occurs from* $\mathbf{x}$ *to* $\mathbf{y}$ *if and only if it occurs from* $\mathbf{y}$ *to* $\mathbf{x}$ *at the same time and the same phase factor.*

Remark 6.1.4. By Theorem 4.1.3(1) and Remark 3.5.4, real vectors with PST are 2-strongly cospectral, so Remark 4.3.4 allows us to say ‘PST between $\mathbf{x}$ and $\mathbf{y}$ at time τ’ in lieu of ‘PST from $\mathbf{x}$ to $\mathbf{y}$ at time τ’. This also follows from Corollary 6.1.3.

We characterise PST between real pure states $\mathbf{x}$ and $\mathbf{y}$ whenever $|\Phi_{\mathbf{x}}| = 2$.

Corollary 6.1.5. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ *with* $\Phi_{\mathbf{x}} = \{\lambda_1, \lambda_2\}$. *The vectors* $\mathbf{x}$ *and* $\mathbf{y}$ *admit perfect state transfer if and only if* $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral. In this case,* $\mathbf{x} = \alpha\mathbf{u}_1 + \beta\mathbf{u}_2$ *and* $\mathbf{y} = \alpha\mathbf{u}_1 - \beta\mathbf{u}_2$ *for some* $\alpha, \beta \in \mathbb{R}\backslash\{0\}$ *with* $\alpha^2 + \beta^2 = \|\mathbf{x}\|^2$ *and unit eigenvectors* $\mathbf{u}_j$ *associated with* λ_j. *The minimum PST time is* $\tau = \frac{\pi}{|\lambda_1 - \lambda_2|}$.

Proof. This follows from Corollary 4.5.1 and Theorem 3.5.12 with $\zeta_\lambda = \pm 1$. The minimum PST time follows from Theorems 3.7.8(1) and 4.4.2(2) with $m = 2$. □

Corollary 6.1.6. *If* X *is a weighted* k*-regular bipartite graph with bipartition* B_1 *and* B_2, *then perfect state transfer occurs between the characteristic vectors* $\mathbf{e}_{B_1}$ *and* $\mathbf{e}_{B_2}$ *in* X, *where* $|B_1| = |B_2|$ *and the minimum PST time is* $\frac{\pi}{2k}$. *That is, if we order the vertices of* X *such that the first* $a = |B_1|$ *vertices belong to* B_1, *then the real pure states*

$$\mathbf{x} = \begin{bmatrix} \mathbf{1}_a \\ \mathbf{0}_a \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} \mathbf{0}_a \\ \mathbf{1}_a \end{bmatrix}$$

admit perfect state transfer in X.

Proof. Since X is bipartite and regular, it is necessary that $|B_1| = |B_2|$. Let $a = |B_1|$ Since X is k-regular, k is an eigenvalue of A with associated unit eigenvector $\mathbf{u}_1 = \frac{1}{\sqrt{2a}}\mathbf{1}_{2a} = \frac{1}{\sqrt{2a}}(\mathbf{e}_{B_1} + \mathbf{e}_{B_2})$. Since X is bipartite, $-k$ is also an eigenvalue of A with eigenvector $\mathbf{u}_2 = \frac{1}{\sqrt{2a}}(\mathbf{e}_{B_1} - \mathbf{e}_{B_2})$. Taking $\alpha = \beta = \sqrt{a/2}$ and $\lambda_1 = -\lambda_2 = k$ in Corollary 6.1.5 yields PST between $\mathbf{x}$ and $\mathbf{y}$ with minimum PST time $\tau = \frac{\pi}{2k}$ relative to A. Finally, the result also applies to $\alpha D + A$ because X is regular. □

Example 6.1.7. Let $X = C_n$, where n is even. Since C_n is 2-regular, Corollary 6.1.6 implies that PST occurs between $\mathbf{e}_0 + \mathbf{e}_2 + \ldots + \mathbf{e}_{n-2} + \mathbf{e}_n$ and $\mathbf{e}_1 + \mathbf{e}_3 + \ldots + \mathbf{e}_{n-3} + \mathbf{e}_{n-1}$ at time $\tau = \frac{\pi}{4}$.

We now utilise Theorem 5.1.1 to obtain the most general characterisation of PST on real pure states whenever $|\Phi_{\mathbf{x}}| \geq 3$.

Corollary 6.1.8. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ *with* $\Phi_{\mathbf{x}} = \{\lambda_1, \ldots, \lambda_r\}$ *for some* $r \geq 3$. *The vectors* $\mathbf{x}$ *and* $\mathbf{y}$ *admit perfect state transfer if and only if* $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral,* $\frac{\lambda_1 - \lambda_j}{\lambda_1 - \lambda_2} = \frac{p_j}{q_j}$ *for each* $j \geq 3$, *where* p_j *and* q_j *are integers such that* $\gcd(p_j, q_j) = 1$, *and one of the following conditions holds.*

1. *If* $\Phi^+_{\mathbf{x},\mathbf{y}} = \{\lambda_1\}$, *then* p_j *and* q_j *are odd for each* $\lambda_j \in \Phi^-_{\mathbf{x},\mathbf{y}}$.
2. *If* $|\Phi^+_{\mathbf{x},\mathbf{y}}| \geq 2$ *with* $\lambda_1, \lambda_2 \in \Phi^+_{\mathbf{x},\mathbf{y}}$, *then for all* $\lambda_j, \lambda_k \in \Phi^-_{\mathbf{x},\mathbf{y}}$ *and* $\lambda_h \in \Phi^+_{\mathbf{x},\mathbf{y}}\backslash\{\lambda_1, \lambda_2\}$,

$$\nu_2(q_j) = \nu_2(q_k) > \nu_2(q_h),$$

where each $\nu_2(q_h)$ *above is absent whenever* $|\Phi^+_{\mathbf{x},\mathbf{y}}|=2$.

Moreover, the minimum PST time is $\frac{\rho}{2}$, *where* ρ *is given in Lemma 3.7.8.*

Proof. Suppose perfect state transfer occurs between $\mathbf{x}$ and $\mathbf{y}$. By Theorem 4.1.3, it must be that $\mathbf{x}$ and $\mathbf{y}$ are m-strongly cospectral. Since $\mathbf{x},\mathbf{y}$ are real vectors, Remark 3.5.4 implies that $m=2$. Hence, we have $E_j\mathbf{x}=e^{2\pi\ell_j/2}$ where $\ell_j=0$ if $\lambda_j\in\Phi^+_{\mathbf{x},\mathbf{y}}$ and $\ell_j=1$ otherwise. By Theorem 5.1.1(1), we may write $\frac{\lambda_1-\lambda_j}{\lambda_1-\lambda_2}=\frac{p_j}{q_j}$ for each $j\geq 2$, where $p_j,q_j\in\mathbb{Z}$ and $\gcd(p_j,q_j)=1$. By Theorem 5.1.1(2), we also have that $\frac{qp_j}{q_j}\equiv\ell_j-\ell_1 \pmod 2$ for each $j\geq 2$, where $q=\operatorname{lcm}(q_2,q_3,\ldots,q_r)$ and $p_2=q_2=1$. In particular, $q\equiv\ell_2-\ell_1 \pmod 2$. If $\Phi^+_{\mathbf{x},\mathbf{y}}=\{\lambda_1\}$, then $\ell_1=0$ and $\ell_j=1$ for all $j\geq 2$. Hence, q is odd and $\frac{qp_j}{q_j}$ is odd for each $j\geq 2$. From this, 1 is straightforward. Now, if $\lambda_1,\lambda_2\in\Phi_{\mathbf{x},\mathbf{y}}$, then $\ell_1=\ell_2=0$, and so q is even. Suppose $\lambda_h\in\Phi^+_{\mathbf{x},\mathbf{y}}\backslash\{\lambda_1,\lambda_2\}$ and $\lambda_j,\lambda_k\in\Phi^-_{\mathbf{x},\mathbf{y}}$ so that $\ell_h=0$ and $\ell_j=\ell_k=1$. Then $\frac{qp_h}{q_h}$ is even and $\frac{qp_j}{q_j},\frac{qp_k}{q_k}$ are odd. The former implies that $\nu_2(q)>\nu_2(q_h)$, while the latter implies that $\nu_2(q)=\nu_2(q_j)=\nu_2(q_k)$. This proves 2. $\square$

Combining Corollary 6.1.8 and Theorem 3.7.10 recovers the characterisation of PST on vertex states due to Coutinho [32, Theorem 2.4.4], which happens to apply to real pure states whose eigenvalue supports have sizes at least three. Such a characterisation can also be derived from Theorem 5.1.2 where $m=2$ and $\ell_1=0$.

Corollary 6.1.9. *Let* $\mathbf{x},\mathbf{y}\in\mathbb{R}^n$ *such that* $|\Phi_{\mathbf{x}}|\geq 3$ *and* $\Phi_{\mathbf{x}}$ *is a set of algebraic integers, closed under algebraic conjugates. Then* $\mathbf{x}$ *and* $\mathbf{y}$ *admit perfect state transfer if and only if all conditions below hold.*

1. *The vectors* $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral.*
2. *Each eigenvalue* $\lambda_j\in\Phi_{\mathbf{x}}$ *is of the form* $\lambda_j=\frac{1}{2}(a+b_j\sqrt{\Delta})$, *where* a, b_j, *and* Δ *are integers and either* $\Delta=1$ *or* $\Delta>1$ *is a square-free natural number.*
3. *Let* $\lambda_1\in\Phi^+_{\mathbf{x},\mathbf{y}}$. *For all* $\lambda_h\in\Phi^+_{\mathbf{x},\mathbf{y}}$ *and* $\lambda_j,\lambda_k\in\Phi^-_{\mathbf{x},\mathbf{y}}$, *we have*

$$\nu_2\left(\frac{\lambda_1-\lambda_h}{\sqrt{\Delta}}\right)>\nu_2\left(\frac{\lambda_1-\lambda_j}{\sqrt{\Delta}}\right)=\nu_2\left(\frac{\lambda_1-\lambda_k}{\sqrt{\Delta}}\right).$$

In the case that there is PST between $\mathbf{x}$ *and* $\mathbf{y}$, *the minimum PST time is* $\frac{\pi}{g\sqrt{\Delta}}$, *where* g *is given in Theorem 3.7.8.*

We close this section with the following result.

Corollary 6.1.10. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ *be linearly independent. For all* $\tau > 0$ *and for all integers* $r_1, r_2 \geq 1$ *such that* $r_1 + r_2 \leq n$*, there exists a real symmetric matrix* M *such that perfect state transfer occurs between* $\mathbf{x}$ *and* $\mathbf{y}$ *relative to* M *at time* τ*,* $|\Phi^+_{\mathbf{x},\mathbf{y}}| = r_1$ *and* $|\Phi^-_{\mathbf{x},\mathbf{y}}| = r_2$*.*

Proof. We modify the proof of Theorem 4.6.3. Set $r = r_1 + r_2$. Since $\mathbf{x}$ and $\mathbf{y}$ are real, we may take $\theta = 0$ in the proof of Theorem 4.6.3. Moreover we may choose

$$\mathbf{z}_1 = \begin{bmatrix} \mathbf{1}_{r_1} \\ \mathbf{0}_{r-r_1} \end{bmatrix} \quad \text{and} \quad \mathbf{z}_2 = \begin{bmatrix} \mathbf{0}_{r-r_2} \\ \mathbf{1}_{r_1} \end{bmatrix}$$

in (4.6.4), and so the orthonormal $\mathcal{U}$ and $\mathcal{V}$ may be taken to be a set of real vectors, and hence Q may be taken to be an orthogonal matrix. From this, it follows that the matrix M in (4.6.9) is real symmetric. This yields PST between $\mathbf{x}$ and $\mathbf{y}$ relative to M at time τ, with $|\Phi^+_{\mathbf{x},\mathbf{y}}| = r_1$ and $|\Phi^-_{\mathbf{x},\mathbf{y}}| = r_2$. ☐

6.2 Strong and weak cospectrality

In this section, we establish characterisations of weak and strong cospectrality for real pure states.

Theorem 6.2.1. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$*. The following are equivalent relative to* M*.*

1. *The pure states* $\mathbf{x}$ *and* $\mathbf{y}$ *are weakly cospectral.*
2. *For all integers* $k \geq 0$*,* $\mathbf{x}^T M^k \mathbf{x} = \mathbf{y}^T M^k \mathbf{y}$*.*
3. *The walk modules* $W_M(\mathbf{x}+\mathbf{y})$ *and* $W_M(\mathbf{x}-\mathbf{y})$ *are orthogonal subspaces of* $\mathbb{R}^n$*.*
4. *There is an orthogonal matrix* Q *such that* $QM = MQ$*,* $Q^2 = I$ *and* $Q\mathbf{x} = \mathbf{y}$*.*

Proof. The equivalence of 1 and 2 follows from Theorem 3.4.6. Since $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, the term $\operatorname{Im}(\mathbf{y}^* M^j \mathbf{x})$ in (3.4.2) is equal to zero for each j. Thus, $W_M(\mathbf{x}+\mathbf{y})$ and $W_M(\mathbf{x}-\mathbf{y})$ are orthogonal if and only if $\mathbf{x}^T M^j \mathbf{x} - \mathbf{y}^T M^j \mathbf{y} = 0$ for each j. Hence, 2 and 3 are equivalent. To finish the proof, we prove that 3 implies 4, and 4 implies 2. Assume 3 holds. Suppose $W_M(\mathbf{x}+\mathbf{y})$ and $W_M(\mathbf{x}-\mathbf{y})$ are orthogonal and let W_0 be the orthogonal complement of $W_M(\mathbf{x}+\mathbf{y}) \oplus W_M(\mathbf{x}-\mathbf{y})$. Now, let Q be the orthogonal matrix such that $Q\mathbf{x} = \mathbf{x}$ for all $\mathbf{x} \in W_M(\mathbf{x}+\mathbf{y}) \oplus W_0$ and $Q\mathbf{x} = -\mathbf{x}$ for all $\mathbf{x} \in W_M(\mathbf{x}-\mathbf{y})$. Clearly, $Q^2 = I$, and because

$$2Q\mathbf{x} = Q((\mathbf{x}+\mathbf{y}) + (\mathbf{x}-\mathbf{y})) = (\mathbf{x}+\mathbf{y}) - (\mathbf{x}-\mathbf{y}) = 2\mathbf{y},$$

we have $Q\mathbf{x} = \mathbf{y}$. Since $Q^2 = I$, we also have $Q\mathbf{y} = \mathbf{x}$. Finally, if $\mathbf{u} \in W_M(\mathbf{x}+\mathbf{y}) \cup W_0$ and $\mathbf{v} \in W_M(\mathbf{x} - \mathbf{y})$, then using the fact that $W_M(\mathbf{x} + \mathbf{y})$, W_0 and $W_M(\mathbf{x} - \mathbf{y})$ are M-invariant, we obtain

$$QM\mathbf{u} = M\mathbf{u} = MQ\mathbf{u} \quad \text{and} \quad QM\mathbf{v} = -M\mathbf{v} = MQ\mathbf{v},$$

from which it follows that $QM = MQ$. This proves 4. Now, suppose 4 is true. Then $M = QMQ$, and because $Q^2 = I$, we get $M^k = QM^kQ$ for all integers $k \geq 0$. Since $Q = Q^{-1} = Q^T$ and $Q\mathbf{x} = \mathbf{y}$, we obtain

$$\mathbf{x}^T M^k \mathbf{x} = \mathbf{x}^T (QM^kQ)\mathbf{x} = (\mathbf{x}^T Q^T) M^k (Q\mathbf{x}) = (Q\mathbf{x})^T M^k (Q\mathbf{x}) = \mathbf{y}^T M^k \mathbf{y}.$$

This proves 3. $\square$

For real pure states, we say that $\mathbf{x}$ and $\mathbf{y}$ are *strongly cospectral* if

$$E_j\mathbf{x} = \pm E_j\mathbf{y}$$

for each j. This allows us to partition $\Phi_{\mathbf{x}}$ into two sets $\Phi^+_{\mathbf{x},\mathbf{y}}$ and $\Phi^-_{\mathbf{x},\mathbf{y}}$ defined in Remark 3.5.4.

Remark 6.2.2. Let $d = |\Phi_{\mathbf{x}}|$. Taking $m = 2$ in Remark 3.5.3, we obtain $2^{d-1} - 1$ vectors $\mathbf{y}$ that are strongly cospectral with $\mathbf{x}$.

The following result characterises strong cospectrality on real pure states. It may be viewed as an extension of a characterisation of strongly cospectral vertices due to Godsil [56, Theorem 10.2].

Theorem 6.2.3. *Let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$. The following are equivalent relative to M.*

1. *The pure states $\mathbf{x}$ and $\mathbf{y}$ are strongly cospectral.*
2. *There exists a nonempty proper subset σ_1 of $\Phi_{\mathbf{x}}$ such that the orthogonal matrix*

   $$Q = \sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} E_\lambda - \sum_{\theta \in \sigma_1} E_\theta$$

   is a polynomial in M satisfying $QM = MQ$, $Q^2 = I$ and $Q\mathbf{x} = \mathbf{y}$.
3. *There exists a nonempty proper subset σ_1 of $\Phi_{\mathbf{x}}$ such that*

   $$\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} \mathbf{u}_\lambda + \sum_{\theta \in \sigma_1} \mathbf{u}_\theta \quad \textit{and} \quad \mathbf{y} = \sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} \mathbf{u}_\lambda - \sum_{\theta \in \sigma_1} \mathbf{u}_\theta,$$

where $\mathbf{u}_\lambda$ *and* $\mathbf{u}_\theta$ *are real eigenvectors associated with the eigenvalues in* $\Phi_{\mathbf{x}}$*.*

Moreover, if 2 or 3 holds, then $\mathbf{x}$ *and* $\mathbf{y}$ *are strongly cospectral with* $\Phi^+_{\mathbf{x},\mathbf{y}} = \Phi_{\mathbf{x}} \backslash \sigma_1$ *and* $\Phi^-_{\mathbf{x},\mathbf{y}} = \sigma_1$*.*

Proof. Let $M = \sum_{\lambda \in \text{spec}} \lambda E_\lambda$ be the spectral decomposition of M. We prove 1 implies 2, 2 implies 3 and 3 implies 1.

To prove 1 implies 2, assume $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ are strongly cospectral. By Theorem 3.5.7, they are weakly cospectral. Thus, by Theorem 6.2.1(4), there is an orthogonal matrix Q such that $QM = MQ$, $Q^2 = I$ and $Q\mathbf{x} = \mathbf{y}$. Recall that $W_M(\mathbf{x}+\mathbf{y})$ is generated by $\{M^j\mathbf{x} : j = 0, 1, \ldots, n-1\}$. Since $M^j(\mathbf{x}+\mathbf{y}) = \sum_{\lambda \in \Phi_{\mathbf{x}}} \lambda^j E_\lambda(\mathbf{x}+\mathbf{y})$ and $E_\lambda \mathbf{x} = \pm E_\lambda \mathbf{y}$, it follows that $W_M(\mathbf{x}+\mathbf{y})$ is generated by

$$\left\{ \sum_{\lambda \in \Phi^+_{\mathbf{x},\mathbf{y}}} \lambda^j E_\lambda \mathbf{x} : j = 0, 1, \ldots, n-1 \right\}.$$

Also, since $ME_\lambda \mathbf{x} = \lambda E_\lambda \mathbf{x}$, it follows that $W_M(\mathbf{x}+\mathbf{y})$ is a direct sum of eigenspaces that correspond to $\Phi^+_{\mathbf{x},\mathbf{y}}$. Using the same argument, $W_M(\mathbf{x}+\mathbf{y})$ is also a direct sum of eigenspaces that belong to $\Phi^-_{\mathbf{x},\mathbf{y}}$. By Theorem 6.2.1(3), $W_M(\mathbf{x}+\mathbf{y})$ and $W_M(\mathbf{x}-\mathbf{y})$ are orthogonal subspaces of $\mathbb{R}^n$. Thus, if $\Phi_0 := \text{spec}(M) \backslash \Phi_{\mathbf{x}}$ is nonempty, then the orthogonal complement W_0 of $W_M(\mathbf{x}+\mathbf{y}) \oplus W_M(\mathbf{x}-\mathbf{y})$ is a direct sum of eigenspaces that belong to Φ_0. Thus, we may take

$$Q = \sum_{\lambda \in \Phi^+_{\mathbf{x},\mathbf{y}} \cup \Phi_0} E_\lambda - \sum_{\theta \in \Phi^-_{\mathbf{x},\mathbf{y}}} E_\theta. \tag{6.2.1}$$

Since each E_λ is a polynomial in M by Proposition 2.3.2, it follows from (6.2.1) that Q is a polynomial in M. Taking $\sigma_1 := \Phi^-_{\mathbf{x},\mathbf{y}}$ establishes 2.

We now prove 2 implies 3. By Proposition 3.3.2, we may write $\mathbf{x} = \sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} \mathbf{u}_\lambda + \sum_{\theta \in \sigma_1} \mathbf{u}_\theta$. Since $Q\mathbf{x} = \mathbf{y}$, we obtain

$$Q\mathbf{x} = \left(\sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} E_\lambda - \sum_{\theta \in \sigma_1} E_\theta \right) \left(\sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} \mathbf{u}_\lambda + \sum_{\theta \in \sigma_1} \mathbf{u}_\theta \right) = \sum_{\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1} E_\lambda \mathbf{u}_\lambda - \sum_{\theta \in \sigma_1} E_\theta \mathbf{u}_\theta = \mathbf{y}.$$

Finally, we prove 3 implies 1. By assumption, $\mathbf{u}_\lambda$ and $\mathbf{u}_\theta$ are real eigenvectors associated with the eigenvalues in $\Phi_{\mathbf{x}}$. Thus, if $\theta \in \sigma_1$, then we get $E_\theta \mathbf{x} = \sum_{\theta \in \sigma_1} E_\theta \mathbf{u}_\theta$ and $E_\theta \mathbf{y} = -\sum_{\theta \in \sigma_1} E_\theta \mathbf{u}_\theta$, from which it follows that $E_\theta \mathbf{x} = -E_\theta \mathbf{x}$. Similarly, if $\lambda \in \Phi_{\mathbf{x}} \backslash \sigma_1$, then $E_\lambda \mathbf{x} = E_\lambda \mathbf{x}$. Thus, $E_\lambda \mathbf{x} = \pm E_\lambda \mathbf{y}$ for all $\lambda \in \Phi_{\mathbf{x}}$ so 1 holds. □

Remark 6.2.4. By replacing $\mathbf{x} = \mathbf{e}_u$ and $\mathbf{y} = \mathbf{e}_v$ in Theorems 6.2.1 and 6.2.3, we respectively recover the characterisations of cospectral and strongly cospectral vertices due to Godsil and Smith (see Theorems 3.1 and 10.2 in [56]).

Remark 6.2.5. Suppose X is a weighted walk-regular graph. For each $\lambda \in \operatorname{spec}(A)$, we have $(E_j)_{u,u} = (E_j)_{v,v}$ for all $u, v \in V(X)$. From Theorem 6.2.1(2), this condition is equivalent to the fact that $A^k \circ I$ is a constant multiple of I for all integers $k \geq 0$.

6.3 Nonnegativity

We now investigate how the nonnegativity property of pure states affect their quantum state transfer properties.

The *covering radius of a set* $S \subseteq V(X)$ is the least nonnegative integer r such that each vertex of X has distance at most r from S. Note that the maximum value of r in X is equal to the diameter of X. Moreover, S is a dominating set if and only if $r = 1$. We also note that if $S = \{u\}$ then the covering radius of S is the eccentricity of vertex u. The *covering radius of a vector* $\mathbf{x} \in \mathbb{R}^n$ is defined as the covering radius of the set

$$S = \{u \in V(X) : \mathbf{x}^T \mathbf{e}_u \neq 0\}.$$

For more about covering radius, see [37, Section 5.2].

We require the following lemma [49, Lemma 4.1].

Lemma 6.3.1. *Suppose* $\mathbf{x} \in \mathbb{R}^n$ *is not a fixed state and has covering radius* r. *If* M *and* $\mathbf{x}$ *are entrywise nonnegative, then* $|\Phi_{\mathbf{x}}| \geq r + 1$.

Remark 6.3.2. If X is a primitive strongly regular graph and $S = \{u, v\}$, where u and v are adjacent, then $r = 2$ but $\mathbf{x} = \mathbf{e}_u - \mathbf{e}_v$ satisfies $|\Phi_{\mathbf{x}}(A)| = 2$. Thus, Lemma 6.3.1 need not hold if $\mathbf{x}$ is not entrywise nonnegative.

Proposition 6.3.3. *If* u *is a non-isolated vertex in* X *and* $n \geq 3$, *then* $|\Phi_{\mathbf{e}_u}| \geq 2$. *If we further suppose that* $\mathbf{e}_u$ *is involved in strong cospectrality, then* $|\Phi_{\mathbf{e}_u}| \geq 3$.

Proof. A non-isolated vertex in a graph has covering radius at least one, so Lemma 6.3.1 yields $|\Phi_{\mathbf{e}_u}| \geq 2$. The second statement follows from [74, Theorem 3.4]. $\square$

An alternate proof for the first statement in Proposition 6.3.3 is as follows. Since X has no isolated vertices, a vertex state $\mathbf{e}_u$ is not an eigenvector for M. Thus, $\mathbf{e}_u$ is not a fixed state by Proposition 3.3.3, which yields $|\Phi_{\mathbf{e}_u}| \geq 2$. Thus, Corollary 6.1.5 does not apply to vertex states, but Corollaries 6.1.8 and 6.1.9 do.

Theorem 6.3.4. *Let M and $\mathbf{x} \in \mathbb{R}^n \backslash \{\mathbf{0}\}$ be entrywise nonnegative.*

1. *If $|\Phi_{\mathbf{x}}| = 2$, then $\mathbf{x}$ is periodic and the covering radius of $\mathbf{x}$ is at most one.*
2. *Suppose $\mathbf{x}$ is periodic relative to M. If $|\Phi_{\mathbf{x}}| \geq 3$ and $\Phi_{\mathbf{x}}$ is a set of real algebraic integers, closed under taking algebraic conjugates, then the covering radius of $\mathbf{x}$ is at most $2k$, where k is the maximum row sum of M.*

Proof. Let r be the covering radius of $\mathbf{x}$. Since M and $\mathbf{x}$ are entrywise nonnegative, Lemma 6.3.1 gives us

$$r + 1 \leq |\Phi_{\mathbf{x}}|. \tag{6.3.1}$$

Combining this with Theorem 3.7.8 (1) yields 1. Next, let λ_1 be the spectral radius of M. Because $|\Phi_{\mathbf{x}}| \geq 3$, $\Phi_{\mathbf{x}}$ is a set of real algebraic integers, closed under taking algebraic conjugates and $\mathbf{x}$ is periodic, Corollary 3.7.18 implies that

$$|\Phi_{\mathbf{x}}| \leq 2\lambda_1 + 1. \tag{6.3.2}$$

Since $\lambda_1 \leq k$, combining (6.3.1) and (6.3.2) yields

$$r + 1 \leq |\Phi_{\mathbf{x}}| \leq 2\lambda_1 + 1 \leq 2k + 1,$$

from which the result in 2 follows. □

Remark 6.3.5. Theorem 6.3.4 applies to A. Further, if we take $M = kI - L$, then any eigenvector for L is an eigenvector for M, and so $\lambda \in \Phi_{\mathbf{x}}$ relative to L if and only if $k - \lambda \in \Phi_{\mathbf{x}}$ relative to L. Consequently, Theorem 6.3.4 also applies to L.

Theorem 6.3.6. *For each $k > 0$, there are only finitely many connected graphs X with positive integer weights and maximum degree at most k such that a real vector $\mathbf{x}$ with nonnegative rational entries is periodic relative to A or L.*

Proof. First, assume that X is a connected unweighted graph with maximum degree k. Suppose $\mathbf{x}$ is a periodic pure state with nonnegative rational entries. By Lemma 3.3.7, $\Phi_{\mathbf{x}}$ is closed under taking algebraic conjugates. Let r be the covering radius of $\mathbf{x}$. Since $\mathbf{x}$ is not fixed, we have $|\Phi_{\mathbf{x}}| \geq 2$, and so applying Theorem 6.3.4 to $M \in \{A, kI - L\}$ yields $r \leq 2k$. This implies that the diameter of X is at most $2k$. Since k is fixed, there are only finitely connected graphs with diameter at most $2k$. This remains true if we assign positive integer weights to X. □

Note that the above theorem remains true for the adjacency matrix even if the graphs in question have loops of positive integer weights, since this condition does not change the fact that $r \leq 2k$ (from Theorem 6.3.4) and the covering radius is at most the diameter of the graph. Since we may represent the adjacency matrices of the class of connected graphs with positive integer weights and maximum degree at most k using irreducible nonnegative matrices with integer entries having maximum row sum at most k, we obtain the following corollary to the above theorem.

Corollary 6.3.7. *For each $k > 0$, there are only finitely many irreducible nonnegative integer matrices M with maximum row sum at most k such that a real vector $\mathbf{x}$ with nonnegative rational entries is periodic relative to M. The matrices M need not be hollow.*

Theorem 6.3.6 generalises Godsil's result on periodic vertex states [51, Corollary 6.2] and Kim et. al's results on periodic s-pair states with nonnegative rational entries [64, Corollary 3.5]. We also note that Theorem 6.3.6 need not apply if $\mathbf{x}$ has a positive and a negative entry; see [80] for instance for an infinite family of trees with maximum degree three admitting PST between pair states.

Remark 6.3.8. The argument in the proof of Theorem 6.3.6 applies when the Hamiltonian taken is $\alpha D + A$, where $\alpha \geq 0$ is an integer. If $\lambda_1(N)$ is the largest eigenvalue of a matrix N, then using the fact that αD and A are nonnegative matrices yields

$$\lambda_1(\alpha D + A) \leq \alpha \lambda_1(D) + \lambda_1(A) \leq (\alpha + 1)k.$$

Thus, we may replace the inequality $r \leq 2k$ in Theorem 6.3.4 by $r \leq 2(\alpha + 1)k$, in which case, we obtain the same result. Lemma 3.3.6 also implies that Theorem 6.3.6 applies to nonnegative vectors $\mathbf{x}$ whenever $a\mathbf{x}$ has rational entries for some $a > 0$.

6.4 Families

In this section, we survey results about PST between real pure states in complete graphs, complete bipartite graphs, cycles, and paths. Since Corollary 6.1.5 takes care of the case $|\Phi_{\mathbf{x}}| = 2$, we only focus on the case when $|\Phi_{\mathbf{x}}| \geq 3$.

The following is immediate from Theorem 5.2.1.

Theorem 6.4.1. *The vectors $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n \backslash \{\mathbf{0}\}$ admit perfect state transfer in K_n relative to $\alpha D + A$ if and only if $\mathbf{x} \notin \operatorname{span}\{\mathbf{1}\}$, $\mathbf{x}$ is not orthogonal to $\mathbf{1}$ and $\mathbf{y} = \mathbf{x} - \frac{2(\mathbf{1}^T\mathbf{x})}{n}\mathbf{1}$. In this case, the minimum PST time is $\frac{\pi}{n}$.*

For the complete bipartite graph $K_{a,b}$, we have the following result relative to A.

Theorem 6.4.2. *Let* $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}, \mathbf{y} \in \mathbb{R}^{a+b}$, *where* $\mathbf{x}_1 \in \mathbb{R}^m$ *and* $|\Phi_{\mathbf{x}}| \geq 3$. *Let* $\mathbf{z}$ *and* $\mathbf{v}^{\pm} = \begin{bmatrix} \sqrt{b}\mathbf{1}_a \\ \pm\sqrt{a}\mathbf{1}_b \end{bmatrix}$ *be eigenvectors for* $A(K_{a,b})$ *associated with 0 and* $\pm\sqrt{ab}$ *respectively. Then* $\mathbf{x}$ *and* $\mathbf{y}$ *admit perfect state transfer in* $K_{m,n}$ *relative to* A *if and only if* $\mathbf{x} \in \operatorname{span}\{\mathbf{v}^+, \mathbf{v}^-, \mathbf{z}\}$, $\mathbf{x} \notin \operatorname{span} \mathcal{W}$ *for any two-subset* $\mathcal{W}$ *of* $\{\mathbf{v}^+, \mathbf{v}^-, \mathbf{z}\}$ *and*

$$\mathbf{y} = \mathbf{x} - 2 \begin{bmatrix} \frac{1}{a}(\mathbf{1}^\top \mathbf{x}_1)\mathbf{1} \\ \frac{1}{b}(\mathbf{1}^\top \mathbf{x}_2)\mathbf{1} \end{bmatrix}.$$

In this case, the minimum PST time is $\tau = \frac{\pi}{\sqrt{ab}}$.

Proof. This follows from Theorem 5.3.1 by taking $m = 2$ and $\tau = \frac{\pi}{\sqrt{ab}}$. ☐

We also state an analogous result for $K_{a,b}$ relative to L.

Theorem 6.4.3. *Let* $\mathbf{x} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \end{bmatrix}, \mathbf{y} \in \mathbb{R}^{a+b}$, *where* $\mathbf{x}_1 \in \mathbb{R}^m$ *and* $|\Phi_{\mathbf{x}}| \geq 3$. *Let* $\mathbf{u}$, $\mathbf{v}$ *and* $\mathbf{w}$ *be eigenvectors for* $L(K_{a,b})$ *associated with* a, b *and* $n = a + b$ *respectively. Then* $\mathbf{x}$ *and* $\mathbf{y}$ *admit perfect state transfer in* $K_{a,b}$ *relative to* L *if and only if* $\mathbf{x} \in \operatorname{span}\{\mathbf{1}, \mathbf{u}, \mathbf{v}, \mathbf{w}\}$, $\mathbf{x} \notin \operatorname{span} \mathcal{W}$ *for any two-subset* $\mathcal{W}$ *of* $\{\mathbf{1}, \mathbf{u}, \mathbf{v}, \mathbf{w}\}$ *and one of the following conditions hold.*

1. $\nu_2(a) = \nu_2(b)$ *and* $\mathbf{y} = \begin{bmatrix} -\mathbf{x}_1 + \frac{2}{a}(\mathbf{1}^T\mathbf{x}_1)\mathbf{1} \\ -\mathbf{x}_2 + \frac{2}{b}(\mathbf{1}^T\mathbf{x}_2)\mathbf{1} \end{bmatrix}$

2. $\nu_2(a) > \nu_2(b)$ *and* $\mathbf{y} = \begin{bmatrix} -\mathbf{x}_1 + \frac{2}{n}((\mathbf{1}^T\mathbf{x}_2) + (\mathbf{1}^T\mathbf{x}_1))\mathbf{1} \\ \mathbf{x}_2 + \frac{2}{n}((\mathbf{1}^T\mathbf{x}_1) - \frac{a}{b}(\mathbf{1}^T\mathbf{x}_2))\mathbf{1} \end{bmatrix}$.

3. $\nu_2(a) < \nu_2(b)$ *and* $\mathbf{y} = \begin{bmatrix} \mathbf{x}_1 + \frac{2}{n}((\mathbf{1}^T\mathbf{x}_2) - \frac{b}{a}(\mathbf{1}^T\mathbf{x}_1))\mathbf{1} \\ -\mathbf{x}_2 + \frac{2}{n}((\mathbf{1}^T\mathbf{x}_1) + (\mathbf{1}^T\mathbf{x}_2))\mathbf{1} \end{bmatrix}$.

The minimum PST time in all cases above is $\frac{\pi}{\gcd(a,b)}$.

Proof. This follows from Theorem 5.3.2 by taking $m = 2$ and $\tau = \frac{\pi}{\gcd(a,b)}$. ☐

Next, we deal with cycles.

Theorem 6.4.4. *Let* $n \geq 3$ *and* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$. *Suppose* $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(A)$ *is closed under algebraic conjugates and* $|\Phi_{\mathbf{x}}| \geq 3$. *Then* C_n *admits perfect state transfer between* $\mathbf{x}$ *and* $\mathbf{y}$ *relative to* $\alpha D + A$ *if and only if one of the following conditions hold.*

1. *$n=2k$, $\mathbf{x}=a\mathbf{v}_0+b(\alpha_1\mathbf{v}_{\frac{n}{6}}+\alpha_2\mathbf{v}_{\frac{5n}{6}})+c(\beta_1\mathbf{v}_{\frac{n}{4}}+\beta_2\mathbf{v}_{\frac{3n}{4}})+d(\gamma_1\mathbf{v}_{\frac{n}{3}}+\gamma_2\mathbf{v}_{\frac{2n}{3}})+e\mathbf{v}_{\frac{n}{2}}$ and $\mathbf{y}=a\mathbf{v}_0-b(\alpha_1\mathbf{v}_{\frac{n}{6}}+\alpha_2\mathbf{v}_{\frac{5n}{6}})+c(\beta_1\mathbf{v}_{\frac{n}{4}}+\beta_2\mathbf{v}_{\frac{3n}{4}})-d(\gamma_1\mathbf{v}_{\frac{n}{3}}+\gamma_2\mathbf{v}_{\frac{2n}{3}})+e\mathbf{v}_{\frac{n}{2}}$, $b\neq 0$ or $d\neq 0$, and either*
   - *(a) If $c=0$, then $k\equiv 0$ (mod 3). In this case $\Phi_{\mathbf{x}}\subseteq\{\pm1,\pm2\}$.*
   - *(b) Else, $k\equiv 0$ (mod 6). Here, $\Phi_{\mathbf{x}}\subseteq\{0,\pm1,\pm2\}$, $0\in\Phi_{\mathbf{x}}$, and $\Phi_{\mathbf{x}}\neq\{0,\pm2\}$.*
2. *$n=4k$, $\mathbf{x}=a\mathbf{v}_0+b(\beta_1\mathbf{v}_k+\beta_2\mathbf{v}_{3k})+c\mathbf{v}_{2k}$ and $\mathbf{y}=-a\mathbf{v}_0+b(\beta_1\mathbf{v}_k+\beta_2\mathbf{v}_{3k})-c\mathbf{v}_{2k}$. In this case $\Phi_{\mathbf{x}}=\{0,\pm2\}$.*
3. *$n=12k$, $\mathbf{x}=a(\alpha_1\mathbf{v}_{3k}+\alpha_2\mathbf{v}_{9k})+b(\beta_1\mathbf{v}_k+\beta_2\mathbf{v}_{11k})+c(\gamma_1\mathbf{v}_{5k}+\gamma_2\mathbf{v}_{7k})$ and $\mathbf{y}=a(\alpha_1\mathbf{v}_{3k}+\alpha_2\mathbf{v}_{9k})-b(\beta_1\mathbf{v}_k+\beta_2\mathbf{v}_{11k})-c(\gamma_1\mathbf{v}_{5k}+\gamma_2\mathbf{v}_{7k})$. Here, $\Phi_{\mathbf{x}}=\{0,\pm\sqrt{3}\}$.*
4. *$n=8k$, $\mathbf{x}=a(\alpha_1\mathbf{v}_{2k}+\alpha_2\mathbf{v}_{6k})+b(\beta_1\mathbf{v}_k+\beta_2\mathbf{v}_{7k})+c(\gamma_1\mathbf{v}_{3k}+\gamma_2\mathbf{v}_{5k})$ and $\mathbf{y}=a(\alpha_1\mathbf{v}_{2k}+\alpha_2\mathbf{v}_{6k})-b(\beta_1\mathbf{v}_k+\beta_2\mathbf{v}_{7k})-c(\gamma_1\mathbf{v}_{3k}+\gamma_2\mathbf{v}_{5k})$. Here, $\Phi_{\mathbf{x}}=\{0,\pm\sqrt{2}\}$.*

In all cases above, $a,b,c,d,e\in\mathbb{R}$ are such that $a^2+b^2+c^2=\|\mathbf{x}\|^2$ in 2-4 with $a,b,c\neq 0$, and $a^2+b^2+c^2+d^2+e^2=\|\mathbf{x}\|^2$ otherwise. Further, $(\alpha_1,\alpha_2),(\beta_1,\beta_2),(\gamma_1,\gamma_2)\in\mathbb{R}^2\backslash\{(0,0)\}$ such that $\alpha_1^2+\alpha_2^2=\beta_1^2+\beta_2^2=\gamma_1^2+\gamma_2^2=1$. The minimum PST time in (1)-(4) is π, $\frac{\pi}{2}$, $\frac{\pi}{\sqrt{3}}$ and $\frac{\pi}{\sqrt{2}}$, respectively.

Proof. We apply Theorem 5.4.2 with $m=2$ and $\ell_1=1$. Since $\mathbf{x},\mathbf{y}$ are real, we may take the scalars a,b,c,d,e and the ordered pairs $(\alpha_1,\alpha_2),(\beta_1,\beta_2),(\gamma_1,\gamma_2)$ in Theorem 5.4.2 as real. In particular, 1(a) and 1(b) follow from Theorem 5.4.2(1a-b), while 2 follows from Theorem 5.4.2(1c) with the vector $\mathbf{x}$ in Theorem 5.4.2(1) reexpressed as $\mathbf{x}=a\mathbf{v}_0+b(\beta_1\mathbf{v}_{\frac{n}{4}}+\beta_2\mathbf{v}_{\frac{3n}{4}})+c\mathbf{v}_{\frac{n}{2}}$ (since $b=d=0$ in this case). Lastly, 3 and 4 follow from Theorem 5.4.2(2-3). □

In Example 5.4.5, we saw examples of real pure states that admit PST in C_8 and C_{12}. We complement these examples by providing instances of PST between real pure states in C_6.

Example 6.4.5. The following hold in C_6.

1. Let $\mathbf{x}=a\mathbf{v}_0+b\mathbf{v}_1+d\mathbf{v}_2+e\mathbf{v}_3$ and $\mathbf{y}=a\mathbf{v}_0-b\mathbf{v}_1-d\mathbf{v}_2+e\mathbf{v}_3$, where $b\neq 0$ and $d\neq 0$. In this case $\Phi_{\mathbf{x}}=\{\pm1,\pm2\}$. Letting $a=e=\frac{\sqrt{n}}{6\sqrt{2}}$ and $b=d=\frac{\sqrt{n}}{\sqrt{2}}$, and applying Theorem 6.4.4(1) with $c=0$, $\alpha_1=\gamma_1=1$ yields PST between $\mathbf{e}_0$ and $\frac{1}{3}(\mathbf{e}_0-2\mathbf{e}_2-2\mathbf{e}_4)$ at time π.

2. Let $\mathbf{x}=a\mathbf{v}_0+b\mathbf{v}_5+d\mathbf{v}_4+e\mathbf{v}_6$ and $\mathbf{x}=a\mathbf{v}_0-b\mathbf{v}_5-d\mathbf{v}_4+e\mathbf{v}_6$. In this case $\Phi_{\mathbf{x}}=\{\pm1,\pm2\}$. Letting $a=-e=\frac{\sqrt{n}}{2\sqrt{2}}$ and $b=d=\frac{\sqrt{n}}{\sqrt{6}}$, and applying

Theorem 6.4.4(1) with $c = 0$, $\alpha_2 = \gamma_2 = 1$ yields PST between $\mathbf{e}_3 + 2\mathbf{e}_1$ and $\mathbf{e}_3 + 2\mathbf{e}_5$ at time π. By reordering the vertices of C_6, this is equivalent to PST between $\mathbf{e}_0 + 2\mathbf{e}_2$ and $\mathbf{e}_0 + 2\mathbf{e}_4$ at time π.

3. By Example 6.1.7, the vectors $\mathbf{e}_0 + \mathbf{e}_2 + \mathbf{e}_4$ and $\mathbf{e}_1 + \mathbf{e}_3 + \mathbf{e}_5$ have PST at $\frac{\pi}{4}$.

The same argument above applied to Theorems 5.5.2 and 5.5.6 yields the following results for paths relative to A and L, respectively.

Theorem 6.4.6. *Let $n \geq 3$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$. Suppose $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(A)$ is closed under algebraic conjugates and $|\Phi_{\mathbf{x}}| \geq 3$. Then P_n admits perfect state transfer between $\mathbf{x}$ and $\mathbf{y}$ relative to A if and only if one of the following conditions hold.*

1. *$n + 1 = 6k$, and either*
   - *(a) $\mathbf{x} = a\mathbf{z}_{3k} + b\mathbf{z}_{2k} + c\mathbf{z}_{4k}$ and $\mathbf{y} = a\mathbf{z}_{3k} - b\mathbf{z}_{2k} - c\mathbf{z}_{4k}$,*
   - *(b) $\mathbf{x} = a\mathbf{z}_{3k} + b\mathbf{z}_{k} + c\mathbf{z}_{5k}$ and $\mathbf{y} = a\mathbf{z}_{3k} - b\mathbf{z}_{k} - c\mathbf{z}_{5k}$, or*
2. *$n + 1 = 4k$, $\mathbf{x} = a\mathbf{z}_{2k} + b\mathbf{z}_{k} + c\mathbf{z}_{3k}$ and $\mathbf{y} = a\mathbf{z}_{2k} - b\mathbf{z}_{k} - c\mathbf{z}_{3k}$.*

In all cases above, $a, b, c \in \mathbb{R}\backslash\{0\}$ are such that $a^2 + b^2 + c^2 = \|\mathbf{x}\|^2$. The minimum PST times in 1a, 1b and 2 are $\frac{\pi}{2}$, $\frac{\pi}{\sqrt{3}}$ and $\frac{\pi}{\sqrt{2}}$, respectively.

Theorem 6.4.7. *Let $n \geq 3$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$. Suppose $\Phi_{\mathbf{x}} = \Phi_{\mathbf{x}}(L)$ is closed under algebraic conjugates and $|\Phi_{\mathbf{x}}| \geq 3$. Then P_n admits perfect state transfer between $\mathbf{x}$ and $\mathbf{y}$ relative to L if and only if one of the following conditions hold.*

1. *$n = 3k$, $\mathbf{x} = a\mathbf{w}_{2k} + b\mathbf{w}_{\frac{3k}{2}} + c\mathbf{w}_{k} + d\mathbf{w}_0$, $\mathbf{y} = -a\mathbf{w}_{2k} + b\mathbf{w}_{\frac{3k}{2}} - c\mathbf{w}_{k} + d\mathbf{w}_0$, and k is even if $b \neq 0$.*
2. *$n = 6k$, $\mathbf{x} = a\mathbf{w}_{3k} + b\mathbf{w}_{5k} + c\mathbf{w}_{k}$ and $\mathbf{y} = a\mathbf{w}_{3k} - b\mathbf{w}_{5k} - c\mathbf{w}_{k}$.*
3. *$n = 4k$, $\mathbf{x} = a\mathbf{w}_{2k} + b\mathbf{w}_{3k} + c\mathbf{w}_{k}$ and $\mathbf{y} = a\mathbf{w}_{2k} - b\mathbf{w}_{3k} - c\mathbf{w}_{k}$.*

In all three cases, $a, b, c, d \in \mathbb{R}$ are such that $a^2 + b^2 + c^2 + d^2 = \|\mathbf{x}\|^2$ in 1 and $a^2 + b^2 + c^2 = \|\mathbf{x}\|^2$ otherwise. The minimum PST times in 2 and 3 are $\frac{\pi}{\sqrt{3}}$ and $\frac{\pi}{\sqrt{2}}$, respectively, and π otherwise.

Next, we determine the forms of real pure states $\mathbf{x}, \mathbf{y}$ and the graphs X such that the minimum PST time between $\mathbf{x}$ and $\mathbf{y}$ in X is the least amongst all unweighted connected n-vertex graphs relative to A and L.

The following result is obtained from Corollary 5.6.2 by taking $m = 2$.

Corollary 6.4.8. *Let* $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$.

1. *Amongst all connected unweighted n-vertex graphs, $\mathbf{x}$ and $\mathbf{y}$ attain the least minimum PST time relative to L if and only if the conditions in Theorem 5.6.1(1) hold and*

$$\mathbf{y} = \frac{1}{n}(\mathbf{1}_n^T\mathbf{x})\mathbf{1}_n - \frac{1}{n_1n_2(n_1+n_2)}\left(\begin{bmatrix} n_2\mathbf{1}_{n_1} \\ -n_1\mathbf{1}_{n_2}\end{bmatrix}^T \mathbf{x}\right)\begin{bmatrix} n_2\mathbf{1}_{n_1} \\ -n_1\mathbf{1}_{n_2}\end{bmatrix}.$$

2. *There exists an integer $N > 0$ such that amongst all connected unweighted n-vertex graphs with $n \geq N$, $\mathbf{x}$ and $\mathbf{y}$ attain the least minimum PST time relative to A if and only if the conditions in Theorem 5.6.1(2) hold and $\mathbf{y}$ has the form below, where $D^{\pm} = \pm a(\lambda^{\pm})\sqrt{(n-a-1)^2+4a(n-a)}$.*

$$\mathbf{y} = \frac{1}{D^-}\left(\begin{bmatrix} -\lambda^-\mathbf{1}_a \\ a\mathbf{1}_{n-a}\end{bmatrix}^T \mathbf{x}\right)\begin{bmatrix} -\lambda^-\mathbf{1}_a \\ a\mathbf{1}_{n-a}\end{bmatrix} - \frac{1}{D^+}\left(\begin{bmatrix} -\lambda^+\mathbf{1}_a \\ a\mathbf{1}_{n-a}\end{bmatrix}^T \mathbf{x}\right)\begin{bmatrix} -\lambda^+\mathbf{1}_a \\ a\mathbf{1}_{n-a}\end{bmatrix}.$$

The minimum PST time in (1) is $\frac{\pi}{n}$. Otherwise, it is $\frac{\pi}{\sqrt{(n-a-1)^2+4a(n-a)}}$ for all sufficiently large n.

7

Vertex state transfer on joins

We devote this and the next chapter to vertex states, which are pure states of the form $\mathbf{e}_u$, where u is a vertex in a graph X. We say that perfect state transfer occurs between vertices u and v in X if their corresponding vertex states $\mathbf{e}_u$ and $\mathbf{e}_v$ admit perfect state transfer. For brevity, we also say vertex PST, in lieu of perfect state transfer between vertex states. We say that vertex u is periodic if $\mathbf{e}_u$ is periodic. In particular, if vertices u and v exhibit PST relative to A (respectively, L), then we also say that u and v admit adjacency PST (respectively, Laplacian PST). Similar language applies to periodicity and strong cospectrality relative to A and L.

Vertex PST has been extensively studied over the last two decades. Our goal in this chapter is to contribute to the existing body of work by addressing vertex PST in join graphs. This chapter is based closely on a joint work of the author with Dr. Stephen Kirkland [66]. The results presented in this chapter are the contributions of the author to this project.

7.1 Joins: motivation

The graphs K_2, C_4 P_3, and $K_4\backslash e$ are well-known examples of small graphs that admit PST relative to $M \in \{A, L\}$. Kirkland et al. noticed that in these small graphs, the vertices involved in perfect state transfer share the same neighbours, an observation that prompted them to examine state transfer between twin vertices [67]. However, it can also be observed that these small graphs are in fact join graphs. This motivates our investigation of quantum walks on graphs built using the join operation.

The first infinite family of join graphs revealed to admit Laplacian perfect state transfer was $K_n\backslash e := O_2 \vee K_{n-2}$ with $n \equiv 0 \pmod 4$ [14]. Motivated by this result, Angeles-Canul et al. gave sufficient conditions for adjacency perfect state transfer to

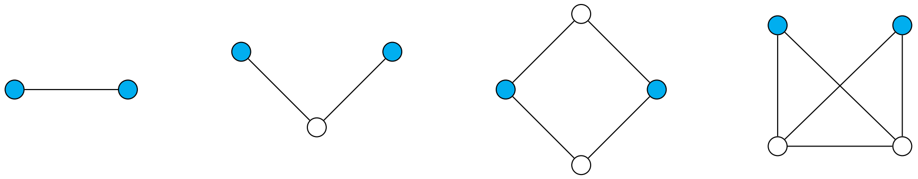

Figure 7.1: Small unweighted graphs that exhibit PST between vertices marked blue

occur between the vertices of $X \in \{O_2, K_2\}$ in the unweighted graph $X \vee Y$, where Y is a regular graph [3] (in this case, $X \vee Y$ is a double cone). In [3] the authors also determined sufficient conditions such that adjacency perfect state transfer in X is preserved under joins of copies of X. In a subsequent paper, Angeles-Canul et al. investigated perfect state transfer in weighted join graphs, and found that the apices of a double cone on a k-regular graph admit adjacency perfect state transfer by appropriate choice of weights of an edge between the apices and/or loops on the apices [2]. More recently, Kirkland et al. fully characterised unweighted double cones that admit adjacency perfect state transfer between apices [67]. For the Laplacian case, Alvir et al. showed that the apices of unweighted $O_2 \vee Y$ admit perfect state transfer if and only if $|V(Y)| \equiv 2 \pmod 4$, while the apices of unweighted $K_2 \vee Y$ do not admit perfect state transfer [1]. Joins were also investigated in graphs with well-structured eigenbases [60, 71] and strong cospectrality [74], as well as in other types of quantum state transfer such as fractional revival [75] and sedentariness [77].

Despite its widespread presence in the literature, state transfer on join graphs remains largely unexplored. Thus, we dedicate this chapter to providing a systematic study of quantum walks on weighted join graphs having the adjacency and Laplacian matrices as the associated Hamiltonians. Throughout, we assume that X and Y are simple weighted graphs on n_1 and n_2 vertices, with the additional assumption that X and Y are weighted k- and ℓ-regular when dealing with $M = A$, respectively.

7.2 Strong cospectrality

In order to avoid confusion, we denote the eigenvalue supports of vertex u in $X \vee Y$ and X by $\Phi_{\mathbf{e}_u}(X \vee Y)$ and $\Phi_{\mathbf{e}_u}(X)$, respectively. Recall that from (3.6.12) that

$$\lambda^{\pm} = \frac{1}{2}(k + \ell \pm \sqrt{\Delta})$$

are eigenvalues of $A(X \vee Y)$, where $\Delta = (k - \ell)^2 + 4n_1n_2$.

We start this section with a result that determines the elements in the eigenvalue supports of vertex states in a join graph. It is immediate from (3.6.10) and (3.6.14).

Lemma 7.2.1. *Let $u \in V(X)$. The following hold.*

1. *Relative to L, we have $\Phi_{\mathbf{e}_u}(X \vee Y) = \{\lambda + n_2 : \lambda \in \Phi_{\mathbf{e}_u}(X) \backslash \{0\}\} \cup \mathcal{R}$, where $\mathcal{R} = \{0, n_1 + n_2\}$ if X is connected and $\mathcal{R} = \{0, n_1 + n_2, n_2\}$ otherwise.*
2. *Relative to A, we have $\Phi_{\mathbf{e}_u}(X \vee Y) = \Phi_{\mathbf{e}_u}(X) \backslash \{k\} \cup \mathcal{R}$, where $\mathcal{R} = \{\lambda^{\pm}\}$ if X is connected and $\mathcal{R} = \{\lambda^{\pm}, k\}$ otherwise.*

Two vertices u and v in X are *strongly cospectral* if their corresponding vertex states $\mathbf{e}_u$ and $\mathbf{e}_v$ are strongly cospectral. That is, if

$$E_j \mathbf{e}_u = \pm E_j \mathbf{e}_v \quad \text{for each } j.$$

Equivalently, for each j, either every eigenvector $\mathbf{w}$ associated with λ_j satisfies $\mathbf{w}^T \mathbf{e}_u = \mathbf{w}^T \mathbf{e}_v$ or every eigenvector $\mathbf{w}$ associated with λ_j satisfies $\mathbf{w}^T \mathbf{e}_u = -\mathbf{w}^T \mathbf{e}_v$. In this case, u and v belong to the same component of X (so neither of them is isolated). By Remark 3.5.4, we may partition $\Phi_{\mathbf{e}_u}(X) = \Phi_{\mathbf{e}_v}(X)$ into two sets:

$$\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{\lambda_j : E_j \mathbf{e}_u = E_j \mathbf{e}_v\} \quad \text{and} \quad \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{\lambda_j : E_j \mathbf{e}_u = -E_j \mathbf{e}_v\}.$$

In order to avoid confusion, if u and v are strongly cospectral in X and $X \vee Y$, then we write the above sets as $\Phi^{\pm}_{\mathbf{e}_u,\mathbf{e}_v}(X)$ and $\Phi^{\pm}_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y)$, respectively.

We are now ready to characterise strong cospectrality in join graphs.

Theorem 7.2.2. *Let $n_1 \geq 2$ and consider two vertices u and v in X.*

1. *Vertices u and v are Laplacian strongly cospectral in $X \vee Y$ if and only if either:*
   - (a) *Vertices u and v are Laplacian strongly cospectral in X and $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. In this case, $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \{\lambda + n_2 : 0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\} \cup \mathcal{R}$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \{\mu + n_1 : \mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)\}$, where $\mathcal{R}$ is given in Lemma 7.2.1(1).*
   - (b) *$X = O_2$. In this case, $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \{0, n_2 + 2\}$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \{n_2\}$.*
2. *Vertices u and v are adjacency strongly cospectral in $X \vee Y$ if and only if either:*
   - (a) *Vertices u and v are adjacency strongly cospectral in X and $\lambda^- \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. In this case, $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \backslash \{k\} \cup \mathcal{R}$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, where $\mathcal{R}$ is given in Lemma 7.2.1(2).*

(b) $X = O_2$. In this case, $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v} = \{\lambda^\pm\}$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v} = \{k\}$.

3. If $w \in V(Y)$, then vertices u and w are not strongly cospectral in $X \vee Y$.

Further, if 1(a) or 2(a) holds, then u and v belong to the same component in X.

Proof. Let λ and μ be nonzero eigenvalues of $L(X)$ and $L(Y)$ with associated eigenvectors $\mathbf{u}_\lambda$ and $\mathbf{v}_\mu$, respectively. From Section 3.6.3, we know that 0, n_1+n_2, $\lambda+n_2$ and $\mu+n_1$ are eigenvalues of L with associated eigenvectors

$$\mathbf{1}_{n_1+n_2}, \quad \mathbf{n} = \begin{bmatrix} n_2\mathbf{1}_{n_1} \\ -n_1\mathbf{1}_{n_2} \end{bmatrix}, \quad \mathbf{x}_\lambda = \begin{bmatrix} \mathbf{u}_\lambda \\ \mathbf{0} \end{bmatrix}, \quad \text{and} \quad \mathbf{y}_\mu = \begin{bmatrix} \mathbf{0} \\ \mathbf{v}_\mu \end{bmatrix} \tag{7.2.1}$$

respectively. Now, let $u, v \in V(X)$. We have two cases.

Case 1. Let u and v be non-isolated in X. From the form of the $\mathbf{x}_\lambda$'s, strong cospectrality in X is required for strong cospectrality in $X \vee Y$. Assume u and v are strongly cospectral in X. If $n_1 \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, then $\mathbf{x}_m$ is another eigenvector for n_1+n_2. Thus, u and v are not strongly cospectral in $X \vee Y$ because $\mathbf{n}^T\mathbf{e}_u = \mathbf{n}^T\mathbf{e}_v$ and $\mathbf{x}_m^T\mathbf{e}_u = -\mathbf{x}_m^T\mathbf{e}_v$. However, if $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, then u and v are strongly cospectral in $X \vee Y$ with $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y)$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y)$ in Theorem 7.2.21(a) as desired.

Case 2. Let u and v be isolated in X. Then $\mathbf{z} = \mathbf{e}_u - \mathbf{e}_v$ is an eigenvector for L associated with the eigenvalue n_2. If $X = O_2$, then [67, Corollary 6.9(2)] yields the desired conclusion. However, if X has a component C other than $\{u\}$ and $\{v\}$, then the vector $\mathbf{w}$ that is constant on each component of X and whose sum of all entries is 0 is also an eigenvector for L associated with the eigenvalue n_2. This vector satisfies $\mathbf{w}^T\mathbf{e}_u = \mathbf{w}^T\mathbf{e}_v$, and since $\mathbf{z}^T\mathbf{e}_u = -\mathbf{z}^T\mathbf{e}_v$, we get that u and v are not strongly cospectral in $X \vee Y$.

Combining the above two cases proves 1. Next, let $\lambda \neq k$ and $\mu \neq \ell$ be eigenvalues of $A(X)$ and $A(Y)$ respectively, with associated eigenvectors $\mathbf{w}_\lambda$ and $\mathbf{z}_\mu$. Then $\lambda^\pm$, λ and μ are eigenvalues of A with associated eigenvectors

$$\begin{bmatrix} (k-\lambda^\mp)\mathbf{1}_{n_1} \\ n_1\mathbf{1}_{n_2} \end{bmatrix}, \quad \mathbf{x}_\lambda = \begin{bmatrix} \mathbf{w}_\lambda \\ \mathbf{0} \end{bmatrix}, \quad \text{and} \quad \mathbf{y}_\mu = \begin{bmatrix} \mathbf{0} \\ \mathbf{z}_\mu \end{bmatrix} \tag{7.2.2}$$

respectively. The same argument as the previous case yields the desired conclusion for 2. Finally, the form of the $\mathbf{x}_\lambda$'s in (7.2.1-7.2.2) yields 3 and the last statement. □

From Theorem 7.2.2(3), we assume henceforth that the strongly cospectral vertices in $X \vee Y$ belong to X.

Example 7.2.3. In the hypercube Q_3, vertices u and v of distance three are strongly cospectral in X with $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(Q_3) = \{1, -3\}$. By Theorem 7.2.22(a), vertices u and v are strongly cospectral in $Q_3 \vee Y$ if and only if $\lambda^- \notin \{1, -3\}$. In particular, if $Y = K_6$, then $\lambda^- = -3$, and so u and v are not strongly cospectral in $Q_3 \vee K_6$.

Corollary 7.2.4. *Let $X \notin \{O_2, K_2\}$ be an unweighted graph. Then vertices u and v in X are Laplacian strongly cospectral in $X \vee Y$ if and only if they are in X.*

Proof. Since X is unweighted, n_1 is an eigenvalue of $L(X)$ if and only if X is a join. From (7.2.1), $n_1 \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ if and only if $n_1 = 2$, in which case $X = K_2$. Combining this with Theorem 7.2.21(a) yields the desired result. $\square$

7.3 Perfect state transfer

To characterise PST in joins, it suffices to consider the vertices of X in checking for PST in $X \vee Y$ by Theorem 7.2.2(3). Throughout, we denote the minimum PST times between u and v in X and $X \vee Y$ by τ_X and $\tau_{X\vee Y}$, respectively. We begin with the Laplacian case. Recall that $\phi(M, t)$ is the characteristic polynomial of M in the variable t and $\nu_2(a)$ is the largest power of two dividing an integer a.

Theorem 7.3.1. *Suppose $n_1 \geq 2$ and $\phi(L(X), t)$ has integer coefficients. Vertices u and v in X admit Laplacian perfect state transfer in $X \vee Y$ if and only if all conditions below hold.*

1. *Either (i) u and v are Laplacian strongly cospectral in X and $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ or (ii) $X = O_2$.*
2. *The eigenvalues in $\Phi_{\mathbf{e}_u}(X)$ are all integers.*
3. *If X is connected, then one of the following conditions hold for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and for all $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$.*
   - *(a) $\nu_2(\lambda) > \nu_2(\mu) = \nu_2(\theta)$ and $\nu_2(n_2) > \nu_2(\mu)$.*
   - *(b) $\nu_2(\mu) > \nu_2(\lambda) = \nu_2(n_2)$.*
   - *(c) $\nu_2(\lambda) = \nu_2(\mu) = \nu_2(n_2)$ and $\nu_2(\lambda + n_2)) > \nu_2(\mu + n_1) = \nu_2(\theta + n_2)$.*

   If $X \neq O_2$ is disconnected, then condition (a) holds (in this case, u and v are in the same component in X). If $X = O_2$, then $n_2 \equiv 2$ (mod 4).

Further, $\tau_{X\vee Y} = \pi/g$, where $g = \gcd(\mathcal{T})$, $\mathcal{T} = \{\lambda + n : \lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{0\}\} \cup \mathcal{R}$ and the set $\mathcal{R}$ is given in Lemma 7.2.1(1).

Proof. From Theorem 7.2.2(1), condition 1 is equivalent to strong cospectrality of u and v in $X \vee Y$. Since $0 \in \Phi_{\mathbf{e}_u}(X \vee Y)$, L is positive semidefinite and $\phi(L(X), t)$ has integer coefficients, Theorem 3.7.10 implies that vertex u is periodic if and only if $\Phi_{\mathbf{e}_u}(X) \subseteq \mathbb{Z}$. Thus, condition 2 is equivalent to periodicity of u and v in $X \vee Y$. Combining this with Corollary 6.1.9 yields PST between u and v in $X \vee Y$ if and only if Corollary 6.1.9(3) holds. To establish (3), suppose X is connected. From Theorem 7.2.21(a), we have

$$\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \{\lambda + n_2 : 0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\} \cup \{0, n_1 + n_2\}$$

and

$$\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X \vee Y) = \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X).$$

Thus, Corollary 6.1.9(3) is equivalent to the condition that

$$\nu_2(\lambda + n_2) > \nu_2(\mu + n_1) = \nu_2(\theta + n_2) \tag{7.3.1}$$

for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. We have three cases.

Case 1. Let $\nu_2(\lambda) > \nu_2(\mu)$ for some $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Since $\nu_2(\lambda + n_2) > \nu_2(\mu + n_1)$ in (7.3.1), $\nu_2(n_2) > \nu_2(\mu)$ for each $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, in which case, $\nu_2(\mu + n_1) = \nu_2(\mu)$. For the equality in (7.3.1) to hold, we need $\nu_2(\mu) = \nu_2(\theta)$ for all $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Hence, $\nu_2(\lambda) > \nu_2(\mu)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. If it happens that $\nu_2(\mu) \geq \nu_2(\eta)$ for some $0 \neq \eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$, then $\nu_2(n_2) > \nu_2(\eta)$, and so $\nu_2(\eta + n) = \nu_2(\eta) \leq \nu_2(\mu) = \nu_2(\mu + n_1)$, a contradiction to (7.3.1). Thus, our assumption in this case combined with (7.3.1) gives us $\nu_2(\lambda) > \nu_2(\mu) = \nu_2(\theta)$ and $\nu_2(n_2) > \nu_2(\mu)$ for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. This establishes 3a.

Case 2. Let $\nu_2(\mu) > \nu_2(\lambda)$ for some $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. If $\nu_2(\lambda) \neq \nu_2(n_2)$, then $\nu_2(\mu + n_1) \geq \nu_2(\lambda + n_2)$, a contradiction to (7.3.1). So, $\nu_2(\lambda) = \nu_2(n_2)$ for each $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$. If it happens that $\nu_2(n_2) \geq \nu_2(\theta)$ for some $\theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, then $\nu_2(\theta + n_2) \neq \nu_2(n_2) = \nu_2(\mu + n_1)$, which contradicts (7.3.1). Therefore, $\nu_2(\mu) > \nu_2(n_2) = \nu_2(\lambda)$ for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. This proves 3b.

Case 3. Let $\nu_2(\mu) = \nu_2(\lambda)$ for some $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. For the strict inequality in (7.3.1) to hold, it is required that $\nu_2(\mu) = \nu_2(\lambda) = \nu_2(n_2)$ for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \cup \{n_1\}$ and $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. From this, we obtain the conditions in 3c.

Combining the above three cases proves 3. Now, if X is disconnected, then $n \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$ by Theorem 7.2.21(b), and so Corollary 6.1.9(3) holds if and only if (7.3.1) holds and $\nu_2(n_2) > \nu_2(\mu + n_1)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Equivalently, 3ai holds. This proves 3b. Finally, if $X = O_2$, then Corollary 6.1.9(3) holds if and only if $\nu_2(n_2 + 2) > \nu_2(n_2)$. Equivalently, $n_2 \equiv 2 \pmod 4$. This proves 3c. The minimum PST time follows from Corollary 6.1.9. □

Remark 7.3.2. If $X \neq K_2$ is unweighted, then we may drop the condition $n_1 \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ in Theorem 7.3.1(1i).

The following result is immediate from Theorem 7.3.1(3).

Corollary 7.3.3. *Suppose $n_1 \geq 2$ and $\phi(L(X), t)$ has integer coefficients. If $n_1 + n_2$ is odd, then $X \vee Y$ has no Laplacian perfect state transfer. Moreover, if n_1 or n_2 is odd and X is either disconnected or admits Laplacian perfect state transfer, then X does not admit Laplacian perfect state transfer in $X \vee Y$.*

A similar argument yields an analogous result for the adjacency case.

Theorem 7.3.4. *Suppose $n_1 \geq 2$, k, ℓ are integers and $\phi(A(X), t)$ has integer coefficients. Vertices u and v in X admit adjacency perfect state transfer in $X \vee Y$ if and only if all of the following conditions hold.*

1. *Either (i) u and v are adjacency strongly cospectral in X and $\lambda^- \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ or (ii) $X = O_2$.*

2. *One of the following conditions hold.*

   (a) *The eigenvalues in $\Phi_{\mathbf{e}_u}(X)$ are all integers and Δ is a perfect square.*

   (b) *X is connected, each $\lambda_j \in \Phi_{\mathbf{e}_u}(X) \backslash \{k\}$ is of the form $\frac{1}{2}(k + \ell + b_j\sqrt{\Delta})$ and $\lambda^\pm = \frac{1}{2}(k + \ell \pm b\sqrt{\Delta})$, where b_j, b, Δ are integers with $b > b_j$ for each j and $\Delta > 1$ is square-free.*

3. *For all $\lambda, \eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \backslash \{k\} \cup \mathcal{R}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, we have*

$$\nu_2\left(\frac{\lambda - \eta}{\sqrt{\Delta}}\right) > \nu_2\left(\frac{\lambda - \mu}{\sqrt{\Delta}}\right) = \nu_2\left(\frac{\lambda - \theta}{\sqrt{\Delta}}\right),$$

   where $\Delta = 1$ whenever 2(a) holds, $\mathcal{R}$ is given in Theorem 7.2.2(2).

Further, $\tau_{X \vee Y} = \frac{\pi}{g\sqrt{\Delta}}$, where $g = \gcd(\mathcal{T})$, $\mathcal{T} = \left\{\frac{\lambda_0 - \lambda}{\sqrt{\Delta}} : \lambda \in \Phi_{\mathbf{e}_u}(X) \backslash \{k\} \cup \mathcal{R}\right\}$, $\mathcal{R}$ is given in Lemma 7.2.1(2) and $\lambda_0 \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v} \backslash \{k\} \cup \mathcal{R}$ is fixed.

Corollary 7.3.5. *If $k+\ell$ is odd, then $X \vee Y$ has no adjacency perfect state transfer.*

Proof. Note that λ^+ and λ^- belong to $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\backslash\{k\} \cup \mathcal{R}$. Thus, if $k+\ell = \lambda^+ + \lambda^-$ is odd, then so is $\lambda^+ - \lambda^-$, a contradiction to Theorem 7.3.4(3). $\square$

In the next two sections, we will utilize Theorems 7.3.1 and 7.3.4 to characterize when vertex PST is preserved and induced in the join.

7.4 PST in X and $X \vee Y$

We now determine when Laplacian PST is preserved in the join.

Corollary 7.4.1. *Suppose $n_1 \geq 2$ and $\phi(L(X), t)$ has integer coefficients. If Laplacian perfect state transfer occurs between vertices u and v in X and $\tau_X = \frac{\pi}{h}$, then it occurs between u and v in $X \vee Y$ if and only if $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ and $\nu_2(\alpha) > \nu_2(h)$ for $\alpha \in \{m, n\}$. In this case, $\tau_{X\vee Y} = \frac{\pi}{g}$, where $g = \gcd(\mathcal{T})$, $\mathcal{T}$ is given in Theorem 7.3.1.*

Proof. If PST occurs between u and v in X, then they are strongly cospectral in X and Theorem 7.3.1(2) holds. Hence, PST occurs in $X \vee Y$ if and only if 1i and 3a of Theorem 7.3.1 holds. Equivalently, $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, $\nu_2(n_1) > \nu_2(\mu)$ and $\nu_2(n_2) > \nu_2(\mu)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. As $\nu_2(h) = \nu_2(\mu) = \nu_2(\mu + n_1)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, these conditions are equivalent to $\nu_2(\alpha) > \nu_2(h)$ for $\alpha \in \{m, n\}$. $\square$

We now give an infinite family of graphs where X and $X \vee Y$ have PST. An $n \times n$ matrix H is called a *Hadamard matrix* if all its entries belong to the set $\{\pm 1\}$ and

$$HH^T = nI.$$

It is known that if an $n \times n$ Hadamard matrix exist, then $n = 2$ or $n \equiv 0 \pmod 4$. Moreover, a Hadamard matrix H is invertible with $H^{-1} = \frac{1}{n}H^T$. For more on Hadamard matrices, see [58]. A graph X is *Hadamard diagonalisable* if its Laplacian matrix is diagonalisable by a Hadamard matrix [9], or equivalently, $L(X) = \frac{1}{n}HDH^T$ for some diagonal matrix D of eigenvalues of $L(X)$.

Example 7.4.2. Let X be a Hadamard diagonalisable graph on $n_1 \geq 4$ vertices with PST between u and v. From [60], $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ respectively consist of integers $\lambda \equiv 0$ and $\mu \equiv 2 \pmod 4$. Since $n_1 \equiv 0 \pmod 4$, Corollary 7.4.1 yields PST between u and v in $X \vee Y$ if and only if $n_2 \equiv 0 \pmod 4$.

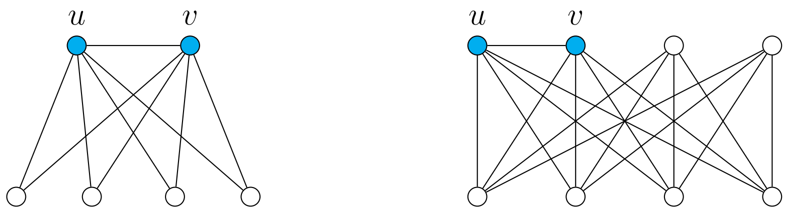

Figure 7.2: Vertices u and v in $K_2 \vee O_4$ (left) are not Laplacian strongly cospectral, while vertices u and v in $(K_2 \cup O_2) \vee O_4$ (right) admit PST

Corollary 7.4.3. *Let X be an unweighted graph on $n_1 = 2^p$ vertices. If Laplacian perfect state transfer occurs between vertices u and v in X, then condition 3a of Theorem 7.3.1 holds. Additionally:*

1. *If $p = 1$, then $X = K_2$ and the graph $K_2 \vee Y$ does not admit Laplacian strong cospectrality between u and v for any Y.*

2. *If $p \geq 2$, then Laplacian perfect state transfer occurs between u and v in $X \vee Y$ if and only if $\nu_2(n) > \nu_2(h)$, where $n = |V(Y)|$ and h is an integer such that $\frac{\pi}{h}$ is the minimum PST time between u and v in X.*

Proof. Assume Laplacian PST occurs between u and v in X. Then Theorem 7.3.1(3) holds. As X is unweighted, each eigenvalue λ of $L(X)$ is at most n_1. Thus, $\nu_2(\lambda) < \nu_2(n_1) = p$, and so conditions 3b and 3c of Theorem 7.3.1 do not hold. Equivalently, condition 3ai holds. From Corollary 7.4.1, PST occurs between u and v in $X \vee Y$ with $\tau_X = \frac{\pi}{h}$ if and only if $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ and $\nu_2(n) > \nu_2(h)$. If $p = 1$, then $X = K_2$ is the only such graph with PST. As $2 \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(L(K_2))$, Theorem 7.2.21(a) yields (1). If $p \geq 2$, then $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, and so (2) holds. □

Corollary 7.4.1 and Theorems 7.2.2(1) and 7.3.1 combined yields our next result.

Corollary 7.4.4. *Let u and v be vertices in X that are strongly cospectral in $X \vee Y$. If $\Phi_{\mathbf{e}_u}(X) \subseteq \mathbb{Z}$ and condition 3a of Theorem 7.3.1 holds, then Laplacian perfect state transfer occurs between u and v in X and $X \vee Y$.*

From Theorem 7.3.1(3a), it is evident that PST in $X \vee Y$ does not necessarily yield PST in X. Thus, the above result can be viewed as a characterisation of the equivalence of PST in a graph and its join.

For a graph X with PST between u and v, it is possible for PST to fail between u and v in $X \vee Y$ for any graph Y, yet occur in $(X \cup Z) \vee Y$ for some graph Z.

Corollary 7.4.5. *Suppose $n_1 \geq 2$ and $\phi(L(X),t)$ has integer coefficients. If Laplacian perfect state transfer occurs between vertices u and v in X and $n_1 \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, then the following conditions hold.*

1. *For any graph Y, Laplacian perfect state transfer does not occur between u and v in $X \vee Y$.*
2. *Let Z be a graph on r vertices such that $n_1 + r \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Then Laplacian perfect state transfer occurs between u and v in $(X \cup Z) \vee Y$ if and only if $\nu_2(n_2) > \nu_2(n_1) = \nu_2(r)$.*

Proof. Since $n_1 \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, we get that u and v are not strongly cospectral in $X \vee Y$ by Theorem 7.2.2(1). This proves 1. We now prove 2. Since $n_1 + r \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, Corollary 7.4.1 implies that PST occurs between u and v in $X \vee Y$ if and only if $\nu_2(n_1 + r) > \nu_2(n_1)$ and $\nu_2(n_2) > \nu_2(n_1)$. Equivalently, $\nu_2(n_2) > \nu_2(n_1) = \nu_2(r)$. $\square$

Example 7.4.6. Let $X = K_2$ with vertices u and v. By Corollary 7.4.3(1) and Theorem 7.3.1, PST between u and v fails in $K_2 \vee Y$ for any graph Y. However, since $r + 2 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(L(K_2))$ for all $r \geq 1$, Corollary 7.4.5 yields PST between u and v in $(K_2 \cup Z) \vee Y$ if and only if $\nu_2(n_2) > \nu_2(r) = 1$. In particular, we may specifically take $Z = O_2$ and $Y = O_4$ (see Figure 7.2).

In contrast with the Laplacian case in Corollary 7.4.5(2), it turns out that if X is regular and has adjacency PST between two vertices, then we can always choose a regular graph Y such that adjacency PST is preserved in $X \vee Y$.

Corollary 7.4.7. *Suppose $n_1 \geq 2$, k, ℓ are integers and $\phi(A(X),t)$ has integer coefficients. If adjacency perfect state transfer occurs between vertices u and v in X and $\tau_X = \frac{\pi}{h}$, then it also occurs between them in $X \vee Y$ if and only if*

1. *$n_2 = \frac{s(k-\ell+s)}{n_1}$ for some integer s such that n_1 divides $s(k-\ell+s)$ and $\ell - s \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, and*
2. *for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, $\nu_2(s) > \nu_2(k-\mu)$ and $\nu_2(\ell - k) > \nu_2(k-\mu)$.*

Here, $\tau_{X \vee Y} = \frac{\pi}{g}$, where $g = \gcd(\mathcal{T})$, $\mathcal{T}$ is given in Theorem 7.3.4, $\lambda_0 \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v} \backslash \{k\} \cup \mathcal{R}$ is fixed and $\nu_2(g) = \nu_2(h)$.

Proof. Suppose perfect state transfer occurs between vertices u and v in X and $\tau_X = \frac{\pi}{h}$. Since k is an integer, Corollary 6.1.9(1) implies that $\Phi_{\mathbf{e}_u}(X) \subseteq \mathbb{Z}$. By Theorem 7.3.4, PST occurs between u and v in $X \vee Y$ if and only if

(a) Δ is a perfect square and $\lambda^- \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, and

(b) For all $\eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\backslash\{k\} \cup \mathcal{R}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, we have

$$\nu_2(\lambda^\pm - \eta) > \nu_2(\lambda^\pm - \mu) = \nu_2(\lambda^\pm - \theta).$$

By the choice of s in (1), $\Delta = (k-\ell)^2+4n_1n_2 = (k-\ell+2s)^2$. Since $\lambda^\pm = \frac{1}{2}(k+\ell\pm\sqrt{\Delta})$, we get $\lambda^+ = k+s$ and $\lambda^- = \ell - s$. Thus, (1) ensures that condition (a) holds. Since X has PST between u and v, Corollary 6.1.9(3) yields

$$\nu_2(k-\eta) > \nu_2(k-\mu) = \nu_2(k-\theta) \tag{7.4.1}$$

for all $\eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\backslash\{k\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Observe that for each $\lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{k\}$, we can write $\lambda^+ - \lambda = (\lambda^+ - k) + (k - \lambda) = s + (k-\lambda)$. Similarly, we have $\lambda^- - \lambda = (\ell - s - k) + (k - \lambda)$. Thus,

$$\nu_2(\lambda^+ - \lambda) \geq \min\{\nu_2(s), \nu_2(k-\lambda)\} \quad \text{and} \quad \nu_2(\lambda^- - \lambda) \geq \min\{\nu_2(\ell-s-k), \nu_2(k-\lambda)\}. \tag{7.4.2}$$

We have the following cases.

Case 1. Suppose $\nu_2(s) > \nu_2(k-\mu)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Combining this with (7.4.2) gives us $\nu_2(\lambda^+ - \mu) = \nu_2(\lambda^+ - \theta) = \nu_2(k - \mu)$. Making use of (7.4.1) and (7.4.2), we get $\nu_2(\lambda^+ - \eta) > \nu_2(k-\mu)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, and so we have $\nu_2(\lambda^+ - \eta) > \nu_2(\lambda^+ - \mu) = \nu_2(\lambda^+ - \theta)$ for all $\eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\backslash\{k\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$.

Case 2. Suppose $\nu_2(s) \leq \nu_2(k-\mu)$ for some $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Using (7.4.1) and (7.4.2), we get $\nu_2(\lambda^+ - \eta) = \nu_2(s) \leq \nu_2(\lambda^+ - \mu)$, which violates condition b.

Consequently, $\nu_2(\lambda^+ - \eta) > \nu_2(\lambda^+ - \mu) = \nu_2(\lambda^+ - \theta)$ for all $\eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\backslash\{k\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ if and only if $\nu_2(s) > \nu_2(k-\mu)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Using this fact and arguing similarly as in the above two cases using (7.4.1) and (7.4.2) yields $\nu_2(\lambda^+ - \eta) > \nu_2(\lambda^+ - \mu) = \nu_2(\lambda^+ - \theta)$ for all $\eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)\backslash\{k\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ if and only if $\nu_2(\ell - k) > \nu_2(k-\mu)$ for all $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Thus, the assumption in (2) is equivalent to condition (b) above, which yields the desired conclusion. ☐

The next example illustrates Corollary 7.4.7 and complements Example 7.4.2.

Example 7.4.8. Let X be a simple integer-weighted Hadamard diagonalisable graph on $m \geq 4$ vertices with PST between vertices u and v. Then $n_1 \equiv 0 \pmod 4$ and X is p-regular for some integer p. From Example 7.4.2, $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$ consists of integers $p - \lambda$, where $\lambda \equiv 0 \pmod 4$, while $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ consists of integers $p - \mu$ such that

$\mu \equiv 2 \pmod 4$. Invoking Corollary 7.4.7(2), we get PST between u and v in $X \vee Y$ if and only if (i) $n_2 = \frac{s(p-\ell+s)}{n_1}$, where s is an integer such that n_1 divides $s(p-\ell+s)$ and $\ell - s \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ and (ii) $\nu_2(s) \geq 2$ and $\nu_2(\ell - p) \geq 2$.

Remark 7.4.9. If $X = K_2$, then $k = -\mu = 1$. Thus, the condition $\ell - s \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ in Corollary 7.4.7(1) is equivalent to $\ell \neq n-1$, while the conditions $\nu_2(s) > 1$ and $\nu_2(\ell - 1) > 1$ in Corollary 7.4.7(2) are equivalent to $\nu_2(s-2) = 1$ and $\nu_2(\ell+3) > 1$. This recovers a characterisation of PST in connected double cones, which are join graphs of the form $K_2 \vee Y$ [67, Theorem 12(1)].

Lastly, we state a characterisation of the equivalence of PST in $X \vee Y$ and X, analogous to Corollary 7.4.4.

Corollary 7.4.10. *Suppose $n_1 \geq 2$, k, ℓ are integers and $\phi(A(X), t)$ has integer coefficients.*

1. *If X is disconnected and perfect state transfer occurs between vertices u and v in $X \vee Y$, then it also occurs between them in X if and only if $X \neq O_2$.*
2. *If X is connected and perfect state transfer occurs between u and v in $X \vee Y$, then it occurs between them in X if and only if the eigenvalues in $\Phi_{\mathbf{e}_u}(X)$ are all integers, Δ is a perfect square and $\nu_2(k-\eta) > \nu_2(k-\mu) = \nu_2(k-\theta)$ for any $\eta \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) \backslash \{k\}$ and $\mu, \theta \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$.*

7.5 PST in $X \vee Y$ but not in X

Under certain assumptions, Laplacian PST can be induced in $X \vee Y$ by appropriate choice of Y. The following results are immediate from Theorem 7.3.1.

Corollary 7.5.1. *Suppose $n_1 \geq 2$, X is connected and $\phi(L(X), t)$ has integer coefficients. If u and v are strongly cospectral vertices in X with $\Phi_{\mathbf{e}_u}(X) \subseteq \mathbb{Z}$ such that the $\nu_2(\mu) > \nu_2(\lambda)$ for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$ and $\mu \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, then:*

1. *Laplacian perfect state transfer occurs between u and v in X, and*
2. *Laplacian perfect state transfer occurs between u and v in $X \vee Y$ if and only if $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, X is connected and $\nu_2(\lambda) = \nu_2(n_1) = \nu_2(n_2)$ for all $0 \neq \lambda \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$.*

We now give an infinite family of graphs such that $X \vee Y$ has PST but not X.

The *cocktail party graph* on $2m$ vertices, denoted by $CP(m)$, is the join of m copies of O_2.

Example 7.5.2. Let $X = CP(m)$, where $m \equiv 2 \pmod 4$. Then $(m-2)$-regular and non-adjacent vertices u and v in X are strongly cospectral with $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{0, m\}$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{m-2\}$ Since $\nu_2(m-2) > \nu_2(n_1)$, Corollary 7.5.1 implies that Laplacian PST does not occur between u and v in X, but it does in $X \vee Y$ if and only if $n_2 \equiv 2 \pmod 4$. In particular, if $n_2 = 2$, then $X \vee Y = CP(m+2)$ admits PST between non-adjacent vertices.

Corollary 7.5.3. *Suppose $n_1 \geq 2$ and $\phi(L(X), t)$ has integer coefficients. Assume u and v are strongly cospectral vertices in X with $\Phi_{\mathbf{e}_u}(X) \subseteq \mathbb{Z}$ such that the $\nu_2(\lambda)$'s are equal for all $0 \neq \lambda \in \Phi_{\mathbf{e}_u}(X)$, say to α. Write each $0 \neq \lambda_r \in \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$ as $\lambda_r = 2^\alpha(2p_r - 1)$ and each $\mu_s \in \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$ as $\mu_s = 2^\alpha(2q_s - 1)$ for some $p_r, q_s \in \mathbb{Z}$. Then Laplacian perfect state transfer occurs between u and v in $X \vee Y$ if and only if X is connected, $n_1 \notin \Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X)$, $\nu_2(n_1) = \nu_2(n_2) = \alpha$ (so we may write $n_1 = 2^\alpha(2y-1)$ and $n_2 = 2^\alpha(2z+1)$ for some $y, z \in \mathbb{Z}$), and one of the following conditions below hold for all r, s, t.*

1. *All $\nu_2(q_s)$s are equal and all of $\nu_2(p_r)$, $\nu_2(y)$ and $\nu_2(z)$ are larger than $\nu_2(q_s)$ for all r, s.*
2. *All $\nu_2(p_r)$'s are equal and $\nu_2(p_r) = \nu_2(y) = \nu_2(z) < \nu_2(q_s)$.*
3. *For all r, s, t, we have $\nu_2(p_r) = \nu_2(q_s) = \nu_2(y) = \nu_2(z)$, $\nu_2(y+z) > \nu_2(q_s+z)$, and $\nu_2(p_r+z) > \nu_2(q_s+z) = \nu_2(q_t+z)$.*

Remark 7.5.4. If X is an unweighted graph that has an odd number of vertices and an odd number of spanning trees, then the matrix-tree theorem implies that all nonzero eigenvalues in $\Phi_{\mathbf{e}_u}(X)$ are odd. Thus, Corollary 7.5.3 may apply with $\alpha = 0$.

Example 7.5.5. Let $X = P_3$ with end vertices u and v. Then $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{0, 3\}$, $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{1\}$. By Corollary 6.1.9(2), u and v do not admit Laplacian PST in X. However, note that u and v are strongly cospectral vertices with $\Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{0, 3\}$ and $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(X) = \{1\}$. Note that $n_1 = 3 \notin \Phi^+_{\mathbf{e}_u,\mathbf{e}_v}(X)$, $\lambda_1 = 3 = 2(2) - 1$ and $\mu_1 = 1 = 2(1) - 1$, and so $\alpha = 0$, $p_1 = y = 2$ and $q_1 = 1$. Thus, if we choose $n_2 = 2z + 1$ for some integer $z = 2\ell$ where ℓ is odd, then Corollary 7.5.3 implies that Laplacian PST occurs u and v in $X \vee Y$ if and only if $n_2 \equiv 1 \pmod 4$. The same conclusion can be made by invoking Corollary 7.5.1(1). In particular, if $Y = O_{4k-3}$, then $X \vee Y = K_{4k} \backslash e$ has PST between u and v.

For the adjacency matrix, we give one scenario where we can induce PST in the join. The following is immediate from Theorem 7.3.4(3).

Corollary 7.5.6. *Suppose $n_1 \geq 2$, k, ℓ are integers and $\phi(A(X), t)$ has integer coefficients. Assume X is connected with strongly cospectral vertices u and v such that $\Phi_{\mathbf{e}_u}(X) \subseteq \mathbb{Z}$ and*

$$\nu_2(\lambda - \eta) > \nu_2(\lambda - \mu) = \nu_2(\lambda - \theta), \tag{7.5.1}$$

for all $\lambda, \eta \in \Phi^{+}_{\mathbf{e}_u,\mathbf{e}_v}(X) \backslash \{k\}$ and $\mu, \theta \in \Phi^{-}_{\mathbf{e}_u,\mathbf{e}_v}(X)$. If (7.5.1) does not hold for $\lambda = k$, then the following hold.

1. *adjacency perfect state transfer does not occur between u and v in X; and*
2. *adjacency perfect state transfer occurs between u and v in $X \vee Y$ if and only if $\lambda^- \notin \Phi^{-}_{\mathbf{e}_u,\mathbf{e}_v}(X)$, Δ is a perfect square and (7.5.1) also holds for all $\lambda \in \{\lambda^{\pm}\}$.*

Example 7.5.7. Let $m \geq 6$ and $X = CP(m)$, where $m \equiv 2 \pmod 4$. From Example 7.5.2, X is connected, $(m-2)$-regular and any pair of non-adjacent vertices u and v in X are strongly cospectral with $\sigma^{+}_{\mathbf{e}_u,\mathbf{e}_v}(A(X)) = \{m-2, -2\}$ and $\sigma^{-}_{\mathbf{e}_u,\mathbf{e}_v}(A(X)) = \{0\}$, but does not admit PST. In this case, $\sigma^{+}_{\mathbf{e}_u,\mathbf{e}_v}(X) \backslash \{k\} = \{-2\}$ and so (7.5.1) holds for all $\lambda, \eta \in \sigma^{+}_{\mathbf{e}_u,\mathbf{e}_v}(X) \backslash \{k\}$ and $\mu, \theta \in \sigma^{-}_{\mathbf{e}_u,\mathbf{e}_v}(X)$. Applying Corollary 7.5.6(2), adjacency PST between u and v in $X \vee Y$ if and only if $\lambda^- \notin \sigma^{-}_{\mathbf{e}_u,\mathbf{e}_v}(X)$, D is a perfect square and (7.5.1) holds for $\lambda \in \{\lambda^{\pm}\}$. The condition that D is a perfect square is equivalent to $n = \frac{z(m-\ell-2+z)}{m}$ for some $z \in \mathbb{Z}$ such that m divides $z(m-\ell-2+z)$. Thus, $\lambda^- = \frac{1}{2}(m-2+\ell-(m-\ell-2+2z)) = \ell - z$ and so the condition $\lambda^- \notin \sigma^{-}_{\mathbf{e}_u,\mathbf{e}_v}(X)$ is equivalent to $\ell - z \neq 0$. Moreover, since $\lambda^+ = m-2+z$, the condition that (7.5.1) holds for $\lambda \in \{\lambda^{\pm}\}$ is equivalent to $\nu_2(m+z) > \nu_2(m-2+z)$ and $\nu_2(\ell - z + 2) > \nu_2(\ell - z)$. Since $m \equiv 2 \pmod 4$, the preceding inequalities are equivalent to $\nu_2(z) = 1$ and $\nu_2(\ell) > 1$. Thus, adjacency PST occurs between u and v in $X \vee Y$ if and only if $n = \frac{z(m-\ell-2+z)}{m}$ for some $z \in \mathbb{Z}$ such that m divides $z(m-\ell-2+z)$, $\ell - z \neq 0$ and $\nu_2(\ell) > \nu_2(z) = 1$. Indeed, $\sigma^{+}_{uv}(A) = \{\lambda^{\pm}, -2\} = \{m+z-2, \ell-z, -2\}$ and $\sigma^{-}_{uv}(A) = \{0\}$ in $X \vee Y$ and conditions 1-3 in Theorem 7.3.4 hold. In particular, if $(\ell, z) = (0, 2)$, then $Y = O_2$ and $X \vee Y = CP(m+2)$ admits PST between u and v.

Lastly, we characterise graphs with isolated vertices that exhibit PST in the join.

Theorem 7.5.8. *Let u, v be isolated vertices in X. Laplacian perfect state transfer occurs between u and v in $X \vee Y$ if and only if $X = O_2$ and $n_2 \equiv 2$ (mod 4).*

The above result follows from Theorems 7.2.21(b) and 7.3.1(3c). Thus, O_2 is the only graph with isolated vertices that exhibits Laplacian PST in the join. This coincides with a known characterisation of Laplacian PST in double cones [1]. For the adjacency case, we have the following result that follows from Theorem 7.3.4.

Theorem 7.5.9. *If u and v are isolated vertices in X, then adjacency perfect state transfer occurs between u and v in $X \vee Y$ if and only if $X = O_2$, Δ is a perfect square and $\nu_2(\lambda^+ - k) = \nu_2(\lambda^- - k)$.*

7.6 Bounds

In the previous section, we see that PST in X need not extend to $X \vee Y$. Thus, we ask, if $u, v \in V(X)$ then how far can $|U_{M(X\vee Y)}(t)_{u,v}|$ be from $|U_{M(X)}(t)_{u,v}|$ as t ranges over $\mathbb{R}$? We answer this question by providing an upper bound for the absolute value of $|U_{M(X\vee Y)}(t)_{u,v}| - |U_{M(X)}(t)_{u,v}|$. To do this, we define

$$\alpha_L(t) = \frac{n_1 e^{-\mathrm{i}tn_2} + n_2 e^{\mathrm{i}tn_1} - (n_1+n_2)}{n_1(n_1+n_2)} \tag{7.6.1}$$

$$\alpha_A(t) = \frac{e^{\mathrm{i}t\lambda^+}(k-\lambda^-)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k-\lambda^+)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}tk}}{n_1} \tag{7.6.2}$$

and

$$T_L = \{2j\pi/g : j \in \mathbb{Z}\} \quad \text{and} \quad T_A = \{t \in \mathbb{R} : e^{\mathrm{i}tk} = e^{\mathrm{i}t\lambda^+} = e^{\mathrm{i}t\lambda^-}\}, \tag{7.6.3}$$

where $g = \gcd(m, n)$ and $\lambda^{\pm} = \frac{1}{2}(k + \ell \pm \sqrt{\Delta})$, where $\Delta = (k-\ell)^2 + 4n_1n_2$. If the context is clear, then we write as $\alpha_M(t)$ and T_M as $\alpha(t)$ and T, respectively. If we add the assumption that k, ℓ are integers and Δ is a perfect square, then we may write $T_A = \{2j\pi/h : j \in \mathbb{Z}\}$, where $h = \gcd(\lambda^+ - k, \lambda^- - k)$.

Now, from (3.6.11) and (3.6.15) respectively, we obtain

$$U_{L(X\vee Y)}(t)_{u,v} = e^{\mathrm{i}tn_1} U_{L(X)}(t)_{u,v} + \frac{1}{n_1+n_2} + \frac{n_2 e^{\mathrm{i}t(n_1+n_2)}}{n_1(n_1+n_2)} - \frac{e^{\mathrm{i}tn_1}}{n_1}. \tag{7.6.4}$$

and

$$U_{A(X\vee Y)}(t)_{u,v} = U_{A(X)}(t)_{u,v} + \frac{e^{\mathrm{i}t\lambda^+}(k-\lambda^-)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k-\lambda^+)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}tk}}{n_1}. \tag{7.6.5}$$

Combining (7.6.4) and (7.6.5) with (7.6.1) and (7.6.2) yields the following.

Lemma 7.6.1. *We have $\alpha_M(t) = 0$ if and only if $t \in T_M$. Moreover, we have $U_{L(X\vee Y)}(t)_{u,v} - e^{\mathrm{i}tn_1} U_{L(X)}(t)_{u,v} = e^{\mathrm{i}tn_1}\alpha_L(t)$ and $U_{A(X\vee Y)}(t)_{u,v} - U_{A(X)}(t)_{u,v} = \alpha_A(t)$. for any $u, v \in V(X)$ and for all t.*

Theorem 7.6.2. *For all* $u, v \in V(X)$ *and for all* t

$$\left| \, U_{L(X \vee Y)}(t)_{u,v} - e^{\mathrm{i}tn_1} U_{L(X)}(t)_{u,v} \, \right| \leq 2/n_1 \tag{7.6.6}$$

with equality if and only if $\nu_2(m) = \nu_2(n)$, *in which case equality holds in (7.6.6) at time* $\tau = j\pi/g$, *where* j *is any odd integer and* $g = \gcd(m, n)$. *In particular, if equality holds in (7.6.6), then*

$$U_{L(X \vee Y)}(\tau)_{u,v} - e^{\mathrm{i}\tau n} U_{L(X)}(\tau)_{u,v} = U_{L(X \vee Y)}(\tau)_{u,v} + U_{L(X)}(\tau)_{u,v} = 2/n_1. \tag{7.6.7}$$

Proof. Combining Lemma 7.6.1 and (7.6.1) yields (7.6.6), with equality if and only if $e^{\mathrm{i}\tau m} = e^{\mathrm{i}\tau n} = -1$ for some $\tau > 0$. Equivalently, $\nu_2(m) = \nu_2(n)$, in which case $\tau = j\pi/g$ for any odd j. From this, (7.6.7) is immediate. □

The following is an analogue of Theorem 7.6.2 for the adjacency case.

Theorem 7.6.3. *For all* $u, v \in V(X)$ *and for all* t,

$$\left| \, U_{A(X \vee Y)}(t)_{u,v} - U_{A(X)}(t)_{u,v} \, \right| \leq 2/n_1 \tag{7.6.8}$$

with equality if and only if there is a time $\tau > 0$ *such that* $\mathrm{e}^{\mathrm{i}\tau\lambda^+} = \mathrm{e}^{\mathrm{i}\tau\lambda^-} = -\mathrm{e}^{\mathrm{i}\tau k}$, *in which case* $\alpha_A(t) = -2\mathrm{e}^{\mathrm{i}\tau k}/m$. *If in addition,* k, ℓ *are integers and* Δ *is a perfect square, then the latter condition yields* $\{k, \lambda^{\pm}\} \subseteq \mathbb{Z}$ *and* $\nu_2(\lambda^+ - k) = \nu_2(\lambda^- - k)$, *in which case* $\tau = j\pi/h$, *where* $h = \gcd(\lambda^+ - k, \lambda^- - k)$ *and* j *is any odd integer.*

Proof. Since $\lambda^{\pm} = \frac{1}{2}(k + \ell \pm \sqrt{\Delta})$, one checks that

$$\begin{aligned} \frac{e^{\mathrm{i}t\lambda^+}(k - \lambda^-)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k - \lambda^+)}{n_1\sqrt{\Delta}} &= \frac{e^{\mathrm{i}t\lambda^+}(k - \ell + \sqrt{\Delta})}{2n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k - \ell - \sqrt{\Delta})}{2n_1\sqrt{\Delta}} \\ &= \frac{e^{it(k+\ell)/2}}{n_1\sqrt{\Delta}} \left[\sqrt{\Delta}\cos(t\sqrt{\Delta}/2) + \mathrm{i}(k - \ell)\sin(t\sqrt{\Delta}/2) \right]. \end{aligned} \tag{7.6.9}$$

Consequently, the following equation holds for all t

$$\left| \frac{e^{\mathrm{i}t\lambda^+}(k - \lambda^-)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k - \lambda^+)}{n_1\sqrt{\Delta}} \right| = \frac{1}{n_1\sqrt{\Delta}} \sqrt{\Delta + ((k - \ell)^2 - \Delta)\sin^2(t\sqrt{\Delta}/2)}. \tag{7.6.10}$$

Since $n_1 n_2 > 0$ and $\Delta = (k - \ell)^2 + 4n_1 n_2$, we get $(k - \ell)^2 - \Delta = -4n_1 n_2 < 0$. Thus, (7.6.10) gives us $\left|\frac{e^{\mathrm{i}t\lambda^+}(k-\lambda^-)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k-\lambda^+)}{n_1\sqrt{\Delta}}\right| \leq \frac{1}{n_1}$. Combining this with (7.6.5) yields

$$\left|U_{A(X\vee Y)}(t)_{u,v} - U_{A(X)}(t)_{u,v}\right| \leq \left|\frac{e^{\mathrm{i}t\lambda^+}(k-\lambda^-)}{n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k-\lambda^+)}{n_1\sqrt{\Delta}}\right| + \frac{1}{n_1} \leq \frac{2}{n_1},$$

which proves (7.6.8). Using the first equality in (7.6.9), we can write (7.6.5) as

$$U_{A(X\vee Y)}(t)_{u,v} - U_{A(X)}(t)_{u,v} = \frac{e^{\mathrm{i}t\lambda^+}(k-\ell+\sqrt{\Delta})}{2n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}t\lambda^-}(k-\ell-\sqrt{\Delta})}{2n_1\sqrt{\Delta}} - \frac{e^{\mathrm{i}tk}}{n_1}.$$

Thus, equality holds in (7.6.8) if and only if there is a time τ such that $e^{\mathrm{i}\tau\lambda^+} = e^{\mathrm{i}\tau\lambda^-} = -e^{\mathrm{i}\tau k}$. In this case, $U_{A(X\vee Y)}(t)_{u,v} - U_{A(X)}(t)_{u,v} = -\frac{2e^{\mathrm{i}tk}}{n_1}$. This implies that $\{k, \lambda^\pm\}$ satisfies the ratio condition. Thus, if k, ℓ are integers and Δ is a perfect square, then we have $\{k, \lambda^\pm\} \subseteq \mathbb{Z}$. Hence, $e^{\mathrm{i}\tau\lambda^+} = e^{\mathrm{i}\tau\lambda^-} = -e^{\mathrm{i}\tau k}$ if and only if $\nu_2(\lambda^+ - k) = \nu_2(\lambda^- - k)$, in which case $\tau = j\pi/g$ for any odd integer j. □

Corollary 7.6.4. *Let $M \in \{A, L\}$. For all $u, v \in V(X)$ and for all t,*

$$\Big|\, |U_{M(X\vee Y)}(t)_{u,v}| - |U_{M(X)}(t)_{u,v}| \,\Big| \leq 2/n_1. \tag{7.6.11}$$

Equality in (7.6.11) holds for $M = L$ at time τ whenever equality holds in (7.6.6) at time τ, $U_{L(X)}(\tau)_{u,v} \in \mathbb{R}$ and either $U_{L(X)}(\tau)_{u,v} \leq 0$ or $U_{L(X)}(\tau)_{u,v} \geq 2/n_1$. Equality in (7.6.11) holds for $M = A$ at time τ if and only if equality holds in (7.6.8) at time τ, $U_{A(X)}(\tau)_{u,v} = |U_{A(X)}(\tau)_{u,v}|e^{\mathrm{i}\tau k}$ and $|U_{A(X)}(\tau)_{u,v}| \geq 2/n_1$.

Proof. For the case $M = L$, applying the triangle inequality to (7.6.6) yields (7.6.11). Using (7.6.7), we get equality in (7.6.11) if and only if

$$\Big|\, |U_{L(X\vee Y)}(\tau)_{u,v}| - |U_{L(X)}(\tau)_{u,v}| \,\Big| = \Big|\, \left|2/n_1 - U_{L(X)}(\tau)_{u,v}\right| - |U_{L(X)}(\tau)_{u,v}| \,\Big| = 2/n_1.$$

Now, for $M = L$, applying triangle inequality to (7.6.8) yields (7.6.11). Making use of Theorem 7.6.3, we get equality in (7.6.11) if and only if $\Big|\, |U_{A(X)}(\tau)_{u,v} - 2e^{\mathrm{i}\tau k}/m\,| - |U_{A(X)}(\tau)_{u,v}| \,\Big| = 2/n_1$. From this, the above result is immediate. □

Corollary 7.6.4 yields the following result, which may be construed as the quantum walks determined by X and $X \vee Y$ relative to $M \in \{A, L\}$ restricted to the vertices of X become equivalent as we increase the number of vertices of X.

Corollary 7.6.5. *Let $M \in \{A, L\}$. For all $u, v \in V(X)$ and for all t,*

$$\left| \, |U_{M(X\vee Y)}(t)_{u,v}| - |U_{M(X)}(t)_{u,v}| \, \right| \to 0 \quad \text{as } n_1 \to \infty.$$

Finally, we demonstrate that the bound in Corollary 7.6.4 is tight for some families graphs. For $u, v \in V(X)$, define

$$F(t)_{u,v} := |U_{M(X\vee Y)}(t)_{u,v}| - |U_{M(X)}(t)_{u,v}|.$$

From Lemma 7.6.1, we may write $F(t)_{u,v} = \left|U_{M(X)}(t)_{u,v} + \alpha_M(t)\right| - |U_{M(X)}(t)_{u,v}|$.

Example 7.6.6. Suppose $X = X_1 \vee X_2$ has n_1 vertices, $u \in V(X_1)$ and $v \in V(X_2)$. From (3.6.11), we have $U_{L(X\vee Y)}(t)_{u,w} = \frac{1}{n_1}\left(1 - e^{\mathrm{i}tn_1}\right)$. Thus, at $\tau = \frac{\pi}{n_1}$, we have $U_{L(X)}(\tau)_{u,v} = 0$. If n_2 is an odd multiple of n_1, then (7.6.1) gives us $\alpha_L(\tau) = -\frac{2}{n_1}$, and so $F(\tau/2)_{u,v} = -\frac{2}{n_1}$.

Example 7.6.7. Let $k \equiv 2 \pmod 4$, $X = K_{k,k}$ and $u, v \in V(X)$ be in different partite sets. Note that X is k-regular with $m = 2k$ vertices. Choose an ℓ-regular graph Y on n vertices such that $n = \frac{z(z+k-\ell)}{2k}$ for some integer z such that k divides z and $z, \ell \equiv 2 \pmod 4$. In this case, $D = (k-\ell)^2 + 8kn = (k - \ell + 2z)^2$, and so $\lambda^+ = k + z$ and $\lambda^- = \ell - z$. Thus, $\nu_2(\lambda^\pm) > \nu_2(k) = 1$. Now, let $g = \gcd(\lambda^+, \lambda^-, k)$ so that $\lambda^\pm/g$ is even. Set $\tau = \frac{\pi}{g}$. Since $K_{k,k} = O_k \vee O_k$, (3.6.11) gives us

$$U_{A(X\vee Y)}(t)_{u,w} = \frac{1}{\sqrt{\Delta}}\left(e^{\mathrm{i}tn_1/2} - e^{-\mathrm{i}tn_1/2}\right).$$

Thus, $U_{A(X)}(\tau)_{u,v} = 0$. But because $e^{i\tau\lambda^+} = e^{i\tau\lambda^-} = -e^{i\tau k} = 1$, Lemma 7.6.1 implies that $U_A(X \vee Y, t)_{u,v} = \alpha_A(t) = 2/m$. Consequently, $F(\tau)_{u,v} = \frac{2}{m}$. For a more specific example, one may take $X = C_4$ ($k = 2$ and $m = 4$) and $Y = C_9$ ($\ell = 2$, $z = 6$ and $n = 9$). In this case, $\lambda^+ = 8$, $\lambda^- = -4$ and $\tau = \frac{\pi}{2}$ (so that u admits PST with another vertex in the same partite set, and so $U_{A(X)}(\tau)_{u,v} = 0$). One then checks that indeed $U_{A(X\vee Y)}(\tau)_{u,v} = \alpha_A(\tau) = \frac{1}{2}(= \frac{2}{m})$, and so $F(\tau)_{u,v} = \frac{1}{2}(= \frac{2}{m})$.

8

Vertex state transfer on blow-ups

In this chapter, we deal with vertex PST on blow-up graphs. While join graphs are ubiquitous in the quantum walks literature, there are only a handful of such papers related to blow-up graphs. In this chapter, we unravel the many interesting spectral, combinatorial and quantum walk properties of blow-up graphs. We will also demonstrate how this graph operation can be used to construct larger graphs with vertex PST. Like join graphs, blow-up graphs, in some cases, can be used to generate infinite families of graphs with perfect state transfer from graphs without perfect state transfer.

This chapter is based closely on joint works of the author with Dr. Stephen Kirkland and Dr. Hiranmoy Pal [78], and with Dr. Bikash Bhattacharjya and Dr. Hiranmoy Pal [12]. The results presented in this chapter are the contributions of the author to these projects.

8.1 Blow-ups: intro and motivation

There are various kinds of 'blow-ups' in graph theory. But here, we consider the more familiar type of blow-up where every vertex of a graph is replaced by an independent set. This variant of the blow-up operation is a special case of the lexicographic product. The *lexicographic product* $X[Y]$ of X and Y is the graph $X[Y]$ obtained by replacing every vertex of X by a copy of Y, and adding all possible edges between the vertices in the copies of Y corresponding to adjacent vertices in X.

In [46], Ge at al. provided sufficient conditions for PST in lexicographic products. Their results about PST in $X[Y]$ required PST in Y. But in our setting, Y is an empty graph which does not exhibit PST, and so their results are not applicable. This is our main motivation for studying quantum state transfer on blow-up graphs.

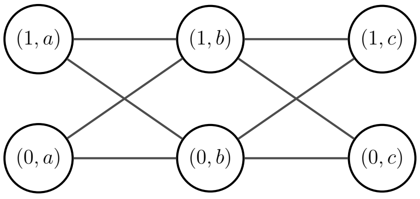

Figure 8.1: The graph $\overset{2}{\uplus} P_3$, a blow-up of two copies of P_3 with vertices a, b, c

Another motivation is to explore a graph operation that induces strong cospectrality between many pairs of vertices, which is promising for the existence of PST. In this section, we endeavour to systematically study quantum state transfer on blow-up graphs relative to A and L. In particular, we focus on the case where X is connected.

A *blow-up* of n copies of a simple weighted graph X, denoted $\overset{n}{\uplus}X$, is the graph with vertex set $\mathbb{Z}_n \times V$ and adjacency matrix

$$A = J_n \otimes A(X).$$

Moreover, the Laplacian matrix of $\overset{n}{\uplus}X$ is given by

$$L = nI_n \otimes D(X) - J_n \otimes A(X).$$

The blow-up of a graph can also be combinatorially defined as follows: $\overset{n}{\uplus}X$ is the graph with vertex set $\mathbb{Z}_n \times V$, and there is an edge between (l, u) and (m, v) in $\overset{n}{\uplus}X$ of weight η if and only if there is an edge between u and v in X of weight η.

Note that $T_u = \{(j, u) : j \in \mathbb{Z}_n\}$ is a false twin set in $\overset{n}{\uplus}X$. If $n \geq 2$, then each vertex in $\overset{n}{\uplus}X$ belongs to a twin set of size at least n_2. In fact, we can say more:

Proposition 8.1.1. *The set $T_u \cup T_v$ is a twin set in $\overset{n}{\uplus}X$ if and only if u and v are false twins in X. In this case, $T_u \cup T_v$ is a false twin set.*

Example 8.1.2. In Figure 8.1, $T_a = \{(0, a), (1, a)\}$ and $T_c = \{(0, c), (1, c)\}$. Since a and c are false twins in P_3, $T_a \cup T_c$ is a false twin set in $\overset{n}{\uplus} P_3$ by Proposition 8.1.1.

The quantum state transfer properties of twin vertices were investigated in a series of papers [67, 74, 75]. We also refer the reader to [73] for a more self-contained treatment of this topic. Since blow-up graphs are graphs with twins, we utilise the results in [67, 74] in characterising perfect state transfer and strong cospectrality in blow-up graphs.

8.2 Transition Matrices

Here, we give a form of the transition matrix of a blow-up graph.

Let λ be an eigenvalue of $A(X)$ associated with the eigenvector $\mathbf{v}$. Then

$$(J_n \otimes A)\left(\mathbf{1} \otimes \mathbf{v}\right) = J_n\mathbf{1} \otimes A\mathbf{v} = n\lambda\left(\mathbf{1} \otimes \mathbf{v}\right).$$

Thus, $n\lambda$ is an eigenvalue of $A(\overset{n}{\uplus}X)$ with eigenvector $\mathbf{1} \otimes \mathbf{v}$. Moreover, since T_u is a twin set in $\overset{n}{\uplus}X$ for each $u \in V(X)$, Lemma 2.2.1 implies that 0 is an eigenvalue of $A(\overset{n}{\uplus}X)$ with multiplicity $(n-1)|V(X)|$. In particular,

$$\left\{\mathbf{e}_{(0,u)} - \mathbf{e}_{(j,u)} : j \in \mathbb{Z}\backslash\{0\}, u \in V(X)\right\}$$

is a linearly independent set of eigenvectors for the eigenvalue 0 of $A(\overset{n}{\uplus}X)$.

Now, let $\operatorname{spec}(A(X)) = \{\lambda_1, \ldots, \lambda_r\}$. First, suppose $0 \in \operatorname{spec}(A(X))$. In this case, we may assume that $\lambda_r = 0$. Then the spectral idempotents of $A(\overset{n}{\uplus}X)$ corresponding to the eigenvalues $n\lambda_1, n\lambda_2, \ldots, n\lambda_{r-1}, \lambda_r = 0$ are respectively given by

$$\frac{1}{n}J_n \otimes E_1, \quad \frac{1}{n}J_n \otimes E_2, \quad \ldots, \quad \frac{1}{n}J_n \otimes E_{r-1}, \quad I_{mn} - \frac{1}{n}J_n \otimes \left(I_m - E_r\right). \tag{8.2.1}$$

Thus, the spectral decomposition of the transition matrix $U_A(t)$ of $\overset{n}{\uplus}X$ given by

$$U_A(t) = \left(\sum_{j=1}^{r-1} e^{\mathrm{i}n\lambda_j t} \cdot \frac{1}{n}J_n \otimes E_j\right) + I_{|V(X)|n} - \frac{1}{n}J_n \otimes \left(I_{|V(X)|} - E_r\right). \tag{8.2.2}$$

On the other hand, if $0 \notin \operatorname{spec}(A(X))$, then we get the same set of spectral idempotents for $A(\overset{n}{\uplus}X)$ in (8.2.1), except for the rth matrix which is now given by $I_{mn} - \frac{1}{n}J_n \otimes I_{|V(X)|}$. This yields the following spectral decomposition of $U_A(t)$:

$$U_A(t) = \left(\sum_{j=1}^{r-1} e^{\mathrm{i}n\lambda_j t} \cdot \frac{1}{n}J_n \otimes E_j\right) + I_{mn} - \frac{1}{n}J_n \otimes I_m.$$

Next, we deal with the Laplacian case. Let λ be an eigenvalue of $L(X)$ associated with the eigenvector $\mathbf{v}$. Note that

$$(nI_n \otimes D - J_n \otimes A)\left(\mathbf{1} \otimes \mathbf{v}\right) = (nI_n \otimes D)(\mathbf{1} \otimes \mathbf{v}) - (J_n \otimes A)(\mathbf{1} \otimes \mathbf{v}) = n\lambda\left(\mathbf{1} \otimes \mathbf{v}\right).$$

Thus, $n\lambda$ is an eigenvalue of $L(\overset{n}{\uplus}X)$ with eigenvector $\mathbf{1} \otimes \mathbf{v}$. Moreover, since T_u is a twin set in $\overset{n}{\uplus}X$, Lemma 2.2.1 implies that $n \deg u$ is an eigenvalue of $A(\overset{n}{\uplus}X)$ with multiplicity $|T_u| - 1$ for each $u \in V(X)$. In particular, for a fixed $u \in V(X)$,

$$\left\{\mathbf{e}_{(0,u)} - \mathbf{e}_{(j,u)} : j \in \mathbb{Z}_n \backslash \{0\}\right\}$$

is a linearly independent set of eigenvectors for the eigenvalue $n \deg u$ of $L(\overset{n}{\uplus}X)$. From this, we get the transition matrix $U_L(t)$ of $\overset{n}{\uplus}X$ as follows:

$$U_L(t) = \sum_{j=1}^{r} e^{\mathrm{i}n\lambda_j t} \left(\frac{1}{n} J_n \otimes E_j\right) + \sum_{u \in V(X)} e^{\mathrm{i}n(\deg u)t} \left(I_n - \frac{1}{n} J_n\right) \otimes \mathbf{e}_u \mathbf{e}_u^T.$$

From this discussion, the following result is immediate.

Proposition 8.2.1. *For any vertex u of X and for all $j \in \mathbb{Z}_n$, we have*

$$\operatorname{spec}\left(M(\overset{n}{\uplus}X)\right) = \{n\lambda : \lambda \in \operatorname{spec}(M(X))\} \cup \mathcal{A}$$

and

$$\Phi_{\mathbf{e}_{(j,v)}} = \{n\lambda : \lambda \in \Phi_{\mathbf{e}_v}(X) \cup \mathcal{B}\},$$

where the sets $\mathcal{A}$ and $\mathcal{B}$ are given by

$$\mathcal{A} = \begin{cases} \{n \cdot \deg u : u \in V(X)\}, & \text{if } M = L \\ \{0\}, & \text{if } M = A \end{cases} \quad \text{and} \quad \mathcal{B} = \begin{cases} \{n \cdot \deg v\}, & \text{if } M = L \\ \{0\}, & \text{if } M = A. \end{cases}$$

For more about the eigenvalues and eigenvectors of blow-up graphs, see [42].

In [35, Lemma 3.3], the authors provided the form of transition matrices of graphs whose adjacency or Laplacian matrices are of the form

$$B \otimes M + C \otimes N,$$

where $\{B, C\}$ and $\{M, N\}$ are pairs of commuting matrices. The adjacency matrix of a blow-up graph obeys the above form, since we may write the matrix $J_n \otimes A$ as $A(K_n) \otimes A + I_n \otimes A$. Despite this fact, the above paper did not have results specific to blow-up graphs. The Laplacian matrix of a blow-up graph, on the other hand, does not have the above form.

We also mention that Monterde investigated sedentariness, a type of low-probability quantum transport, on several variants of the blow-up operation [77]. Apart from this work and that of Ge et al. [46], we are unaware of other results about quantum state transfer on blow-up graphs.

8.3 Strong Cospectrality

We state Corollaries 3.9(2), 3.10 and 3.14 in [67] as one lemma. This can be viewed as a characterisation of strong cospectrality between twin vertices.

Lemma 8.3.1. *Let* $M = \alpha D + A$ *and* T *be a twin set in* X*.*

1. *No vertex in* T *is strongly cospectral with a vertex in* $V(X)\backslash T$*.*
2. *Consider* θ *in Lemma 2.2.1. Two vertices* u *and* v *in* T *are strongly cospectral if and only if either* θ *is a simple eigenvalue of* M *or any eigenvector* $\mathbf{w} \notin \operatorname{span}\{\mathbf{e}_u - \mathbf{e}_v\}$ *associated with* θ *satisfies* $\mathbf{w}^T\mathbf{e}_u = \mathbf{w}^T\mathbf{e}_v = 0$*. Moreover, if* u *and* v *are strongly cospectral, then* $\Phi^-_{\mathbf{e}_u,\mathbf{e}_v}(M) = \{\theta\}$*.*
3. *If* $|T| \geq 3$*, then no vertex in* T *is involved in strong cospectrality in* X*.*

We utilise Lemma 8.3.1 to characterise strong cospectrality in blow-up graphs.

Theorem 8.3.2. *Let* X *be a graph with vertex* u*. The following hold.*

1. *If* $n \geq 3$*, then* $\overset{n}{\uplus} X$ *does not exhibit strong cospectrality.*
2. *Let* $n = 2$*. Then* $(0, u)$ *and* $(1, u)$ *are strongly cospectral in* $\overset{2}{\uplus} X$ *if and only if* $\mu \notin \Phi_{\mathbf{e}_u}(X)$*, where*

   $$\mu = \begin{cases} \deg u, & \text{if } M = L \\ 0, & \text{if } M = A. \end{cases} \tag{8.3.1}$$

   In this case,

   $$\Phi^+_{\mathbf{e}_u,\mathbf{e}_v} = \{n\lambda : \lambda \in \Phi_{\mathbf{e}_v}(X)\} \quad \text{and} \quad \Phi^+_{\mathbf{e}_u,\mathbf{e}_v} = \{n\mu\}$$

   Moreover, $(0, u)$ *is only strongly cospectral with* $(1, u)$ *in* $\overset{2}{\uplus} X$*.*

Proof. If $n \geq 3$, then we have $|T_u| \geq 3$ in $\overset{n}{\uplus} X$ for every vertex u of X. Since T_u is a twin set in $\overset{n}{\uplus} X$, Lemma 8.3.1(3) yields 1. On the other hand, if $n = 2$, then invoking Lemma 8.3.1(2), we get that $\mathbf{e}_0 \otimes \mathbf{e}_u$ and $\mathbf{e}_0 \otimes \mathbf{e}_u$ are strongly cospectral if and only if $\mu \notin \Phi_{\mathbf{e}_u}(X)$. This proves the first statement in 2, while the second statement follows from statements 1 and 2 of Lemma 8.3.1. □

Example 8.3.3. Let X be a weighted tree that has a perfect matching. Since $A(X)$ is invertible if and only if X has a (unique) perfect matching, it follows that $\mu = 0 \notin \Phi_{\mathbf{e}_u}(X)$. Thus, each vertex of $\overset{2}{\uplus} X$ pairs up with a unique vertex to exhibit strong cospectrality relative to A by Corollary 8.3.2(2).

Example 8.3.3 applies to P_{2n}. For P_{2n+1}, we have the following observation.

Example 8.3.4. Let $X = P_{2n+1}$ with edges $\{u, u+1\}$ for each $u \in \{1, \ldots, 2n\}$. Note that 0 is a simple eigenvalue of $A(X)$ with eigenvector $\mathbf{e}_1 - \mathbf{e}_3 + \mathbf{e}_5 - \cdots + (-1)^n \mathbf{e}_{2n+1}$. Therefore, $0 \notin \Phi_{\mathbf{e}_u}(X)$ if and only if u is even. By Theorem 8.3.2(2), $(0, u)$ and $(1, u)$ are strongly cospectral in $\overset{2}{\uplus} X$ relative to A if and only if u is even.

For d-regular graphs, Corollary 8.3.2(2) yields the following.

Corollary 8.3.5. *Let X be a weighted d-regular graph with vertex u. Vertices $(0, u)$ and $(1, u)$ are strongly cospectral in $\overset{2}{\uplus} X$ relative to L if and only if $d \notin \Phi_{\mathbf{e}_u}(X)$. In particular, vertices $(0, u)$ and $(1, u)$ are strongly cospectral in: (i) $\overset{2}{\uplus} K_{d+1}$ for all $d \geq 1$, (ii) $\overset{2}{\uplus} C_n$ if and only if $n \not\equiv 0$ (mod 4), and (iii) $\overset{2}{\uplus} Q_d$ if and only if d is odd.*

8.4 Periodicity

The following result characterises periodicity in blow-up graphs relative to A. It follows from the fact that $0 \in \Phi_{\mathbf{e}_{(j,u)}}$ for all $(j, u) \in V(\overset{n}{\uplus} X)$ and by taking $\theta = 0$ in Corollary 3.7.13(1).

Theorem 8.4.1. *Suppose $n \geq 2$ and $\phi(A(X), t)$ has integer coefficients. Then $\overset{n}{\uplus} X$ is periodic at each $(j, u) \in T_u$ if and only if the elements in $\Phi_{\mathbf{e}_u}(X)$ are all integer multiples of $\sqrt{\Delta}$, where $\Delta \geq 1$ is a square-free integer. In this case, $\rho_{(j,u)} = \frac{2\pi}{g\sqrt{\Delta}}$, where $g = \gcd\{\frac{\lambda}{\sqrt{\Delta}} : \lambda \in \Phi_{\mathbf{e}_u}(X) \backslash \{0\})\}$. Moreover, periodicity in T_u implies periodicity of u in X, and the period of the vertices in T_u is $\frac{\rho}{n}$. Furthermore, if a vertex in T_u is periodic in $\overset{n}{\uplus} X$ for some n, then it is periodic in $\overset{n}{\uplus} X$ for all $n \geq 2$.*

Theorem 8.4.1 implies that the blow-up operation yields shorter periods than the original graph, in contrast with Cartesian products, where the period is at least the period of underlying graphs.

Next, we illustrate that periodicity of u need not yield periodicity in T_u.

Example 8.4.2. Let Y be a k-regular graph on n_2 vertices. Let $X = O_1 \vee Y$ where $V(O_1) = \{u\}$. Then $\Phi_{\mathbf{e}_u}(X) = \{\frac{1}{2}(k \pm \sqrt{k^2 + 4n_2})\}$, and so u is periodic in X at $\tau = \frac{2\pi}{\sqrt{k^2+4n_2}}$ by Theorem 3.7.8(1). Since $0 \notin \Phi_{\mathbf{e}_u}(X)$, Theorem 8.4.1(2) implies that all vertices in T_u are periodic if and only if $k^2 + 4n_2$ is a perfect square or $k = 0$. In both cases, the vertices in T_u are periodic at τ/n.

If $k > 0$ and $k^2 + 4n_2$ is not a perfect square in Example 8.4.2, then any vertex in T_u is not periodic. Thus, blow-ups need not preserve periodicity for the adjacency case. For the Laplacian case, the following is immediate from Theorem 3.7.17.

Corollary 8.4.3. *Suppose* $\deg u$ *is an integer and* $\phi(L(X),t)$ *has integer coefficients. Vertex* (j,u) *in* $\overset{n}{\uplus} X$ *is periodic relative to* L *for some* $n \geq 1$ *if and only if* $\Phi_{\mathbf{e}_u}(X) \subset \mathbb{Z}$. *Moreover, if* $\overset{n}{\uplus} X$ *is periodic at vertex* (j,u) *for some* $n \geq 1$*, then* $\overset{n}{\uplus} X$ *is periodic at vertex* (j,u) *for all* $n \geq 1$ *and* $j \in \mathbb{Z}_n$ *with* $\rho_{(j,u)} = \frac{2\pi}{nh}$*, where* $h = \gcd(\Phi_{\mathbf{e}_u}(X) \backslash \{0\} \cup \{\deg u\})$.

Unlike the adjacency case, Theorem 3.7.17 and Corollary 8.4.3 imply that blow-up graphs preserve Laplacian periodicity.

Proposition 8.4.4. *Let* $M \in \{A, L\}$ *and suppose* $\phi(M,t)$ *has integer coefficients.*

1. *Let* $M = A$. *For all* $n \geq 2$*, the adjacency quantum walk on* X *is periodic at* $\rho = \frac{2\pi}{g\sqrt{\Delta}}$ *if and only if the quantum walk on* $\overset{n}{\uplus} X$ *is periodic at* $\frac{\rho}{n}$*, where* $\Delta \geq 1$ *is a square-free integer and* $g = \gcd\{\frac{\lambda}{\sqrt{\Delta}} : \lambda \in \operatorname{spec}(A(X))\}$.
2. *Let* $M = L$ *and suppose* $\deg u$ *is an integer. For all* $n \geq 2$*, the Laplacian quantum walk on* X *is periodic at* $\rho_X = \frac{2\pi}{g}$ *if and only if* $\overset{n}{\uplus} X$ *is periodic at* $\rho_{\overset{n}{\uplus} X} = \frac{g\rho}{nh}$*, where* $g = \gcd(\operatorname{spec}(L(X) \backslash \{0\})$ *and* $h = \gcd(\operatorname{spec}(L(X) \backslash \{0\} \cup \{\deg u : u \in V(X)\})$.

Proof. Suppose X is periodic at τ. Since $0 \in \operatorname{spec}(L)$ and the trace of A is zero, it follows that $\operatorname{spec}(M(X)) = \{b_j\sqrt{\Delta}\}$ by Corollary 3.7.13, where $\Delta \geq 1$ is a square-free integer and we allow $\Delta = 1$ in case $\operatorname{spec}(M(X)) \subseteq \mathbb{Z}$. From Proposition 8.2.1, we have $\operatorname{spec}(M(\overset{n}{\uplus} X)) = \{nb_j\sqrt{\Delta}\} \cup \mathcal{A}$, where $\mathcal{A} = \{0\}$ whenever $M = A$ and $\mathcal{A} = \{n \deg u : u \in V(X)\}$ whenever $M = L$. Thus, for $M = A$, it is clear that $e^{\mathrm{i}tb_j\sqrt{\Delta}} = e^{\mathrm{i}tb_\ell\sqrt{\Delta}}$ holds if and only if $e^{\mathrm{i}(t/n)nb_j\sqrt{\Delta}} = e^{\mathrm{i}(t/n)nb_\ell\sqrt{\Delta}}$. This establishes the forward direction for $M = A$. Now, for $M = L$, Corollary 3.7.13(1) implies that $\Delta = 1$. Thus, $\operatorname{spec}(L(X)) \subseteq \mathbb{Z}$, in which case $\operatorname{spec}(L(\overset{n}{\uplus} X)) \subseteq \mathbb{Z}$. Thus, the quantum walk on $\overset{n}{\uplus} X$ is periodic by Theorem 3.7.3. The converses are straightforward, and the minimum periods are immediate from Proposition 8.2.1 and Theorem 3.7.8. $\square$

Taken together, our results in this section imply that the blow-up operation under mild conditions yields shorter periods as we take more copies of the underlying graph.

8.5 Perfect state transfer

We first state a characterisation of PST between twin vertices in [67, Theorem 11].

Theorem 8.5.1. *Suppose* $\phi(M,t)$ *has integer coefficients and let* $\{u,v\}$ *be a twin set in* X *such that* u *and* v *are strongly cospectral. Perfect state transfer occurs between* u *and* v *if and only if both conditions below hold.*

1. *Each* $\lambda_j \in \Phi^{+}_{\mathbf{e}_u,\mathbf{e}_v}$ *can be written as* $\lambda_j = \theta + b_j\sqrt{\Delta}$*, where each* b_j *is an integer,* $\Delta \geq 1$ *is a square-free integer and* θ *in Lemma 2.2.1 is an integer.*
2. *All the* $\nu_2(b_j)$*'s are equal.*

If, in addition, perfect state transfer occurs between u *and* v*, then the minimum PST time is* $\tau = \frac{\pi}{g\sqrt{\Delta}}$*, where* $g = \gcd(b_j)_{j\geq 1}$*.*

We now characterise PST in blow-up graphs. By virtue of Theorem 8.3.2, we restrict to the case $n = 2$, and it suffices to consider the case where $0 \notin \Phi_{\mathbf{e}_u}(X)$ and $\deg u \notin \Phi_{\mathbf{e}_u}(X)$ whenever $M = A$ and $M = L$, respectively.

Theorem 8.5.2. *Let* $u \in V(X)$ *with* $\mu \notin \Phi_{\mathbf{e}_u}(X)$*, where* μ *is given in (8.3.1). If* $\phi(M,t)$ *has integer coefficients and* $\deg u$ *is an integer whenever* $M = L$*, then the following are equivalent relative to* $M \in \{A, L\}$*.*

1. *Perfect state transfer occurs between* $(0,u)$ *and* $(1,u)$ *in* $\overset{2}{\uplus}\, X$ *at time* τ *with the phase factor* $\gamma = -e^{2i\tau\mu}$*.*
2. *There exists* $\tau \in \mathbb{R}$ *so that* $e^{2i\lambda_j\tau} = -e^{2i\tau\mu}$ *for each* $\lambda_j \in \Phi_{\mathbf{e}_u}(X)$*.*
3. *Vertex* u *is periodic in* X *at time* 2τ *with phase factor* $\gamma = -e^{\mathrm{i}2\tau\mu}$ *for any* $\lambda_j \in \Phi_{\mathbf{e}_u}(X)$*.*
4. *Each* $\lambda_j \in \Phi_{\mathbf{e}_u}(X)$ *can be written as* $\lambda_j = b_j\sqrt{\Delta}$*, where* b_j *is an integer,* $\Delta = 1$ *or* $\Delta > 1$ *is a square-free integer,* $\Delta = 1$ *whenever* $M = L$ *and the* $\nu_2(b_j - \mu)$*'s are all equal.*

If, in addition, perfect state transfer occurs between $(0,u)$ *and* $(0,v)$*, then the minimum PST time is* $\tau = \frac{\pi}{2g\sqrt{\Delta}}$*, where* $g = \gcd(b_j - \mu)_{j\geq 1}$*.*

Proof. By Theorem 4.1.3, PST occurs between u and v if and only if they are strongly cospectral in $\overset{2}{\uplus}\, X$ and

$$\gamma = e^{\mathrm{i}2\tau\lambda_j} = -e^{\mathrm{i}2\tau\mu}$$

for each $\lambda_j \in \Phi_{\mathbf{e}_v}(X)$. Thus, 1 and 2 are equivalent. The above equation also implies that 2 and 3 are equivalent. Finally, equivalence of 1 and 4, as well as the minimum PST time are immediate from Theorem 8.5.1. □

Remark 8.5.3. In Theorem 8.5.2(4), the condition that the $\nu_2(\lambda - \deg u)$'s are equal for all $\lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{0\}$ whenever $M = L$ is equivalent to the condition that $\nu_2(\deg u) < \nu_2(\lambda)$ for all $\lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{0\}$.

Corollary 8.5.4. *Suppose* $\phi(L(X))$ *has integer coefficients and* $u \in V(X)$ *such that* $\deg u$ *is an odd integer. Perfect state transfer occurs in* $\overset{2}{\uplus}\ X$ *between vertices* $(0,u)$ *and* $(1,u)$ *if and only if* $\Phi_{\mathbf{e}_u}(X)$ *consists of even integers.*

Remark 8.5.5. The above theorem applies to integer-weighted regular graphs with odd degree whose eigenvalues are all even integers.

8.6 Common families

Recall that $\operatorname{spec}(A(K_n)) = \{n-1, -1\}$. Thus, the eigenvalues of $A(K_n)$ are all odd if and only if n is even. Invoking Theorem 8.5.2, we obtain the following result.

Corollary 8.6.1. $\overset{2}{\uplus}\ K_n$ *exhibits PST at* $\frac{\pi}{2}$ *if and only if* n *is even.*

For paths and cycles, we have the following result.

Theorem 8.6.2. *Let* $M \in \{A, L\}$ *and* $n \geq 3$*. The following hold.*

1. $\overset{2}{\uplus}\ P_n$ *admits perfect state transfer relative to* A *if and only if (i)* $n = 3$*, between* $(0,2)$ *and* $(1,2)$ *at* $\tau = \frac{\pi}{2\sqrt{2}}$*, or (ii)* $n = 5$*, between* $(0,3)$ *and* $(1,3)$ *at* $\tau = \frac{\pi}{2\sqrt{3}}$*. Moreover,* $\overset{2}{\uplus}\ P_n$ *does not admit perfect state transfer relative to* L *for all* $n \geq 3$*.*
2. $\overset{2}{\uplus}\ C_n$ *does not admit perfect state transfer for all* $n \geq 3$*.*

Proof. First, note that each $\lambda \in \operatorname{spec}(A(X))$ satisfies $-2 < \lambda < 2$. Let r be the covering radius of vertex u. Thus, if u is periodic in X, then combining Corollary 3.7.18, Lemma 6.3.1 and Theorem 6.3.4 yields $r + 1 \leq |\Phi_{\mathbf{e}_u}(X)| \leq 3$. Thus, $r \leq 2$, which implies $n \in \{3, 4, 5\}$. By inspection, we get PST if and only if 1(i) or (1ii) holds. Now, relative to L, the same argument yields $n \in \{3, 4, 5\}$. Using the Laplacian eigenvalues of P_n in Lemma 5.5.5 and Theorem 3.7.3, we get a periodic vertex in this case if and only if $n = 3$. Since periodicity is required for PST, Corollaries 6.1.9 and 8.4.3 imply that $\overset{2}{\uplus}\ P_n$ has no PST for all $n \geq 4$. Now, the only vertices strongly cospectral in $\overset{2}{\uplus}\ P_3$ are $(0,2)$ and $(1,2)$, in which case $\Phi^{+}_{\mathbf{e}_{(0,2),(1,2)}}(L(\overset{2}{\uplus}\ P_3)) = \{0, 3\}$ and $\Phi^{-}_{\mathbf{e}_{(0,2),(1,2)}}(L(\overset{2}{\uplus}\ P_3)) = \{2\}$. Since these two sets violate Theorem 8.5.2(4), we conclude that $\overset{2}{\uplus}\ P_n$ does not have PST for all $n \geq 3$. The same argument can be used to prove the result in 2. $\square$

We now look at PST in the blow-up of a cone $O_1 \vee X$, where X is a k-regular graph on n vertices. Note that the blow-up of a cone can be expressed as $O_2 \vee \overset{2}{\uplus}\ X$, which is a (disconnected) double cone on a $2k$-regular graph on $2n$ vertices. Disconnected double cones over regular graphs were characterised in [67, Theorem 11(1)]. This yields a characterisation of PST in blow-ups of cones over regular graphs.

Theorem 8.6.3. *Let X be a cone on an unweighted k-regular graph on n vertices with apex u. Perfect state transfer occurs between $(0,u)$ and $(1,u)$ in $\overset{2}{\uplus} X$ if and only if either (i) $k=0$ or (ii) $k>0$ and $n=\frac{1}{4}s\,(2k+s)$ for some even integer s such that $\nu_2(2k)>\nu_2(s)$. Moreover, PST occurs at time $\tau=\frac{\pi}{2\sqrt{n}}$ whenever $k=0$ and $\tau=\pi/g$ otherwise, where $g=\gcd(2k,s)$.*

Proof. If u is the apex of X, then $\Phi_{\mathbf{e}_u}(X)=\{\frac{1}{2}(k\pm\sqrt{\Delta})\}$, where $\Delta=k^2+4n$, and so $\mu=0\notin\Phi_{\mathbf{e}_u}$. If $k=0$, then $\Phi_{\mathbf{e}_u}(X)=\{\pm\sqrt{n}\}$. Invoking Theorem 8.5.2(4) yields the desired conclusion in (i). However, if $k>0$, then for Theorem 8.5.2(4) to hold, k^2+4n is a perfect square. Equivalently, $n=\frac{1}{4}s\,(2k+s)$ for some even integer s. This yields $\lambda^+=2k+s$ and $\lambda^-=s$, and so $\nu_2(\lambda^+)=\nu_2(\lambda^-)$ if and only if $\nu_2(2k)>\nu_2(s)$. Applying Theorem 8.5.2(4) yields (ii). $\square$

We illustrate the above theorem with the following example.

Example 8.6.4. Let X be a cone on a k-regular graph H with n vertices.

1. If $H=O_n$, then $k=0$ and $X=K_{1,n}$. By Theorem 8.6.3(1), PST occurs between $(0,u)$ and $(1,u)$ in $\overset{2}{\uplus} X$ at $\frac{\pi}{2\sqrt{n}}$ for all $n\geq 1$.
2. For all $n\geq 3$, let $H=C_n$ and $k=2$. If $n+1$ is a perfect square, then $n=\frac{1}{4}s(2k+s)$ if and only if $s=2(\pm\sqrt{n+1}-1)$. Invoking Theorem 8.6.3(1), we get PST between $(0,u)$ and $(1,u)$ in $\overset{2}{\uplus} X$ if and only if n is odd.

We close this section with the following discussion. For blow-up graphs, PST in $\overset{2}{\uplus} X$ only occurs between vertices at distance two. Nonetheless, we may construct relatively sparse graphs using blow-up graphs, with the property that PST occurs between vertices that are far apart. We illustrate this via Cartesian products.

Example 8.6.5. Suppose $\overset{2}{\uplus} X$ has PST between u and v at time $\tau=\frac{\pi}{g}$. Denote the hypercube of dimension d by Q_d, which is known to be a sparse graph that admits PST between vertices x and y that are at distance d. If g is an even integer, then $(\overset{2}{\uplus} X)\Box Q_d$ has PST between (u,x) and (v,y) for all $d\geq 2$ at time $\frac{\pi}{2}$.

Example 8.6.6. From Example 8.6.4(1), we know $\overset{2}{\uplus} K_{1,m}$ admits PST, say between vertices u and v, at time $\frac{\pi}{2\sqrt{m}}$ for all odd $m\geq 1$. Let $X=P_3^{\Box n}$, which is known to admit PST between vertices x and y that are at distance $2n$. If $m=2n^2$, then $(\overset{2}{\uplus} X)\Box X$ has PST between (u,x) and (v,y) at time $\frac{\pi}{\sqrt{2}}$.

8.7 Regular graphs

We construct infinite families of regular graphs whose blow-ups admit PST. Since the blow-up of a regular graph is regular, the results here apply to both A and L.

An integer-weighted Hadamard diagonalisable graph X on n vertices is known to be d-regular for some integer d. Moreover, all eigenvalues in $\operatorname{spec}(L(X))$ are even integers and $n \equiv 0 \pmod 4$ [9]. Combining this with Corollary 8.5.4 and Remark 8.5.5 yields the next result.

Corollary 8.7.1. *Suppose $\phi(L(X))$ has integer coefficients. If X is a d-regular Hadamard diagonalisable graph for some odd integer d, then perfect state transfer occurs in $\overset{2}{\uplus} X$ between $(0,u)$ and $(1,u)$ for any vertex u of X at $\frac{\pi}{2}$.*

Remark 8.7.2. Not all Hadamard diagonalisable graphs with odd degree admit PST. A small example is K_4. Nonetheless, the construction in Corollary 8.7.1 applies to any Hadamard diagonalisable graph odd degree. Thus, a blow-up graph can have PST even if the underlying graph does not have PST.

Next, we use Cartesian products to obtain infinite families of blow-up graphs where every vertex pairs up a unique vertex to exhibit PST.

Theorem 8.7.3. *Let $X = X_1 \square \cdots \square X_d$, where each X_j is k_j-regular and $k = k_1 + \cdots + k_d$ is odd. If $\operatorname{spec}(L(X_j))$ consists of even integers for each j, then perfect state transfer occurs in $\overset{2}{\uplus} X$ between $(0,u)$ and $(1,u)$ for any vertex u of X at $\frac{\pi}{2}$.*

Proof. First, note that X is k-regular. Since $\operatorname{spec}(X_j)$ consists of even integers for each $j \in \{1,\dots,d\}$, (3.6.1) implies that the eigenvalues in $\operatorname{spec}(L(X))$ are all even. As k is odd, invoking Corollary 8.5.4 and Remark 8.5.5 yield the desired result. $\square$

The *Hamming graph*, denoted $H(d,q)$, is the Cartesian product of d copies of K_q.

Corollary 8.7.4. *If $X = K_{n_1} \square \cdots \square K_{n_d}$, where each $n_j \geq 2$ is even and $d \geq 2$ is odd, then perfect state transfer occurs in $\overset{2}{\uplus} X$ between $(0,u)$ and $(1,u)$ for any vertex u of X. In particular, if q is even, then perfect state transfer occurs in $\overset{2}{\uplus} H(d,q)$ between $(0,u)$ and $(1,u)$ for any vertex u of $H(d,q)$.*

Proof. Since $\operatorname{spec}(L(K_{n_j})) = \{0, n_j\}$ consists of even integers for all $j \in \{1,\dots,d\}$, letting $X_j = K_{n_j}$ and $k_j = n_j - 1$ in Theorem 8.7.3 yields the first statement. The second statement follows from the first by taking $n_1 = \cdots = n_d = q$ to be even. $\square$

Since $H(2,d) = Q_d$, the second statement of Corollary 8.7.4 together with Corollary 8.3.5(iii) implies that $\overset{2}{\uplus}\, Q_d$ admits PST if and only if d is odd. In this case, PST occurs between vertices $(0,u)$ and $(1,u)$ for any vertex u of Q_d at time $\frac{\pi}{2}$.

Next, we use direct products to construct infinite families of blow-ups with PST.

Theorem 8.7.5. *Let* $X = X_1 \times \cdots \times X_d$ *such that* X_j *is regular and* $\operatorname{spec}(A(X_j)) \subseteq \mathbb{Z}$ *for each* j*. For each* j*, suppose the* $\nu_2(\lambda)$*'s are equal for all* $\lambda \in \operatorname{spec}(A(X_j))$*. Then perfect state transfer occurs in* $\overset{2}{\uplus}\, X$ *between* $(0,u)$ *and* $(1,u)$ *for any vertex* u *of* X*.*

Proof. Our assumption that for each j, $\operatorname{spec}(A(X_j))$ consists of integers with equal largest power of two dividing them implies that 0 is not an adjacency eigenvalue of each X_j. From (3.6.6), we get that the adjacency eigenvalues θ_r of X have equal largest power of two dividing them. Thus, $\theta_r \neq 0$ for all r, and so $\lambda_r = k - \theta_r \neq k$ for all r. Moreover, since X is k-regular for some k, each Laplacian eigenvalue $\lambda_r \in \operatorname{spec}(L(X))$ can be written as $\theta_r = k - \lambda_r$, which we know have equal largest power of two dividing them. Invoking Theorem 8.5.2(4) yields the desired conclusion. □

Corollary 8.7.6. *If* $X = K_{n_1} \times \cdots \times K_{n_d}$*, where each* $n_j \geq 2$ *is even, then perfect state transfer occurs in* $\overset{2}{\uplus}\, X$ *between* $(0,u)$ *and* $(1,u)$ *for any vertex* u *of* X*.*

Proof. As each n_j is even, the adjacency eigenvalues -1 and $n_j - 1$ of K_{n_j} are odd integers. Applying Theorem 8.7.5 with $X_j = K_{n_j}$ for each j yields the result. □

Next, we have the following result that is immediate from Theorem 8.7.5.

Corollary 8.7.7. *Let* Y *be a regular non-bipartite graph such that* $\operatorname{spec}(A(Y)) \subseteq \mathbb{Z}$ *and the* $\nu_2(\lambda)$*'s are equal for all* $\lambda \in \operatorname{spec}(A(Y))$*. If* $X = K_2 \times Y$*, then perfect state transfer occurs in* $\overset{2}{\uplus}\, X$ *between* $(0,u)$ *and* $(1,u)$ *for any* $u \in V(Y)$*.*

In Corollary 8.7.7, taking $Y = K_n$ for even n_2 yields an infinite family of blow-ups of bipartite doubles where each vertex pairs up with a unique vertex to exhibit PST.

8.8 Join graphs

Let X and Y be graphs on n_1 and n_2 vertices, respectively. Since

$$\overset{2}{\uplus}\,(X \vee Y) = (\overset{2}{\uplus}\, X) \vee (\overset{2}{\uplus}\, Y),$$

the blow-up of a join is simply the join of the blow-ups of the underlying graphs. In this section, we construct blow-up graphs that have PST using the join operation. We only focus on the case $M = L$.

Theorem 8.8.1. *Suppose $\phi(L(X))$ has integer coefficients and $u \in V(X)$ such that $\deg u$ is an integer and $\deg u \notin \Phi_{\mathbf{e}_u}(X)$. Then perfect state transfer occurs in $\overset{2}{\uplus}\,(X \vee Y)$ between $(0,u)$ and $(1,u)$ if and only if $\Phi_{\mathbf{e}_u}(X) \subset \mathbb{Z}$ and one of the following conditions hold.*

1. *X is connected, and $\nu_2(\lambda + n_2)$ and $\nu_2(n_1 + n_2)$ are larger than $\nu_2(\deg u + n_2)$ for all $\lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{0\}$.*
2. *X is disconnected, u is not an isolated vertex in X, and $\nu_2(\lambda + n_2)$, $\nu_2(n_1 + n_2)$ and $\nu_2(n_2)$ is larger than $\nu_2(\deg u + n_2)$ for all $\lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{0\}$.*

Proof. Let u be a vertex of X such that $\deg u \notin \Phi_{\mathbf{e}_u}(X)$. Define $S = \{\lambda + n_2 : \lambda \in \Phi_{\mathbf{e}_u}(X)\backslash\{0\}\}$. From Lemma 7.2.1(1), we have $\Phi_{\mathbf{e}_u}(X \vee Y) = S \cup \{0, n_1 + n_2\}$ whenever X is connected, and $\Phi_{\mathbf{e}_u}(X \vee Y) = S \cup \{0, n_1 + n_2, n\}$ otherwise. Now, the degree of vertex u in $X \vee Y$ is $\deg u + n_2$. We have two cases. First, suppose X is connected. If $X \neq K_1$, then $0 < \deg u < n_1$ and so $n_2 < \deg u + n_2 < n_1 + n_2$. Since $\deg u \notin \Phi_{\mathbf{e}_u}(X)$, we get that $\deg u + n_2 \notin \Phi_{\mathbf{e}_u}(X \vee Y)$. Meanwhile, if $X = K_1$ (which is connected), then $\deg u + n_2 = n_2 \notin \Phi_{\mathbf{e}_u}(X \vee Y) = \{0, n_1 + n_2\}$. Applying Theorem 8.5.2(4) to both cases yields the desired result in 1. Now, suppose X is disconnected. If u is not isolated, then $\deg u + n_2 \notin \Phi_{\mathbf{e}_u}(X \vee Y)$ because $\deg u \notin \Phi_{\mathbf{e}_u}(X)$, and so Theorem 8.5.2(4) yields the desired result in 2. On the other hand, if u is isolated, then $\deg u + n_2 = n_2 \in \Phi_{\mathbf{e}_u}(X \vee Y)$. By Theorem 8.3.2(2), vertices $(0,u)$ and $(1,u)$ are not strongly cospectral in $\overset{2}{\uplus}\,(X \vee Y)$, and so they do not admit PST. Therefore, u is not an isolated vertex in X if $(0,u)$ were to admit PST in $\overset{2}{\uplus}\,(X \vee Y)$. $\square$

Theorem 8.8.1 yields the following result.

Corollary 8.8.2. *Let $u \in V(X)$ such that $\deg u$ is an integer. The following hold.*

1. *If X is connected and $\operatorname{spec}(L(X)) \cup \{n_1, n_2\} \subset \mathbb{Z}$ consists of odd integers, then perfect state transfer occurs in $\overset{2}{\uplus}\,(X \vee Y)$ between $(0,u)$ and $(1,u)$ if and only if $\deg u$ is even.*
2. *If $\operatorname{spec}(L(X)) \cup \{n_1, n_2\} \subset \mathbb{Z}$ consists of even integers, then perfect state transfer occurs in $\overset{2}{\uplus}\,(X \vee Y)$ between $(0,u)$ and $(1,u)$ if and only if $\deg u$ is odd.*

Proof. The first statements in 1 and 2 are immediate from Theorem 8.8.1(1), while the second statement in 2 is immediate from Theorem 8.8.1(2). If the second statement in 1 holds, then $\nu_2(n_2) > \nu_2(\deg u + n_2)$ by Theorem 8.8.1(2), which is a contradiction because both n_2 and $\deg u + n_2$ are odd. Thus, 1 and 2 hold. $\square$

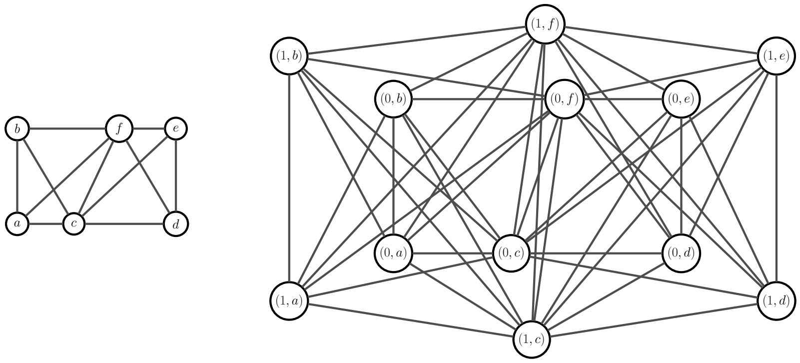

Figure 8.2: The graph $X \vee Y$ where $X = O_1 \vee (K_2 \cup K_2)$ and $Y = O_1$ (left); the graph $\overset{2}{\uplus}(X \vee Y)$ with vertex PST between $(0, u)$ and $(1, u)$ for any vertex u of $X \vee Y$ (right)

For a Hadamard diagonalisable graph X, $\operatorname{spec}(L(X)) \cup \{n_1\}$ consists of even integers. Thus, Corollary 8.8.2 gives us the following result.

Corollary 8.8.3. *Suppose $\phi(L(X))$ has integer coefficients and d is an integer. If X is a d-regular Hadamard diagonalisable graph, then perfect state transfer occurs in $\overset{2}{\uplus}(X \vee Y)$ between $(0, u)$ and $(1, u)$ if and only if d is odd and n_2 is even. In this case, perfect state transfer occurs between $(0, u)$ and $(1, u)$ for any vertex u of X.*

In the next example, $X \cup Y$ denotes the disjoint union of two graphs X and Y.

Example 8.8.4. Let $X = O_1 \vee (K_2 \cup K_2)$. Then $\operatorname{spec}(L(X)) = \{0, 3, 5\}$ and each vertex of X has even degree. As X is connected, Corollary 8.8.2 implies that for all odd n_2, perfect state transfer occurs in $\overset{2}{\uplus}(X \vee Y)$ between $(0, u)$ and $(1, u)$ for any $u \in V(X)$. In particular, if $H = O_1$, then $\overset{2}{\uplus}(X \vee Y)$ admits PST (see Figure 8.2).

If $X = K_1$ in Theorem 8.8.1(1) and $V(K_1) = \{u\}$, then $n_1 = 1$ and $\Phi_{\mathbf{e}_u}(X \vee Y) = \{0, n_2 + 1\}$. Since the largest power of two dividing $\nu_2(n_2 + 1) > \nu_2(\deg u + n_2) = \nu_2(n_2)$ if and only if n_2 is odd, we get the following result.

Corollary 8.8.5. *Let $|V(H)| = n$. If $X = K_1 \vee H$ and $V(K_1) = \{u\}$, then perfect state transfer occurs in $\overset{2}{\uplus} X$ at $\frac{\pi}{2}$ between $(0, u)$ and $(1, u)$ if and only if n is odd.*

Letting $H = O_n$ in Corollary 8.8.5 yields the following result.

Corollary 8.8.6. *$\overset{2}{\uplus} K_{1,n}$ has perfect state transfer between vertices of degree $2n$ if and only if n is odd.*

8.9 Edge perturbation

Throughout this section, we assume that $M = L$ and $n \equiv 0 \pmod 4$. As $n \geq 3$ in this case, $\overset{n}{\uplus}X$ does not exhibit strong cospectrality by Theorem 8.3.2(1), and so $\overset{n}{\uplus}X$ does not admit PST. However, we show that the addition of an appropriate matching in $\overset{n}{\uplus}X$ results in PST. To do this, we need the following result due to Pal [79, Theorem 4]. For a weighted graph with false twins u and v, we let $X(\eta)$ denote the graph resulting from X by adding an edge between u and v of weight η.

Theorem 8.9.1. *Suppose X is a weighted graph and T is a false twin set in X with $u, v \in T$. If u is periodic in X at time τ, then $X(\eta)$ admits PST between u and v whenever $2\eta\tau$ is an odd multiple of π. Moreover, if w is another vertex in X that is periodic, then it remains periodic in $X(\eta)$.*

Now, let u be a vertex in X with $\Phi_{\mathbf{e}_v}(X) \subset \mathbb{Z}$. By Corollary 8.4.3, $\overset{n}{\uplus}X$ is periodic at the vertex (j, u) for all j and n with period $\frac{2\pi}{n}$. Since $n \equiv 0 \pmod 4$, we have that vertex (j, u) is periodic in $\overset{n}{\uplus}X$ for all j at time $\tau = \frac{\pi}{2}$ by Remark 3.7.6. Using the fact that T_u consists of false twins in $\overset{n}{\uplus}X$, Theorem 8.9.1 implies that the insertion of an additional edge in $\overset{n}{\uplus}X$ of weight $\eta = 1$ between vertices $(a, u), (b, u) \in T_v$ with $a \neq b$ results in PST between (a, u) and (b, u) at $\frac{\pi}{2}$. Moreover, the resulting graph is periodic at the remaining vertices in the set $T = \{(j, u) \mid j \neq a, b\}$ with period at time $\frac{\pi}{2}$. Again invoking Theorem 8.9.1, another edge can be added between a pair of vertices in T to have PST at time $\frac{\pi}{2}$. Applying this process inductively, we generate new graphs exhibiting admitting PST by simply adding a *matching* in T_u, which is a set of edges without common vertices. We summarise this as follows.

Theorem 8.9.2. *Let $n \equiv 0$ (mod 4) and u be a vertex in X with $\Phi_{\mathbf{e}_u}(X) \subset \mathbb{Z}$. The addition of a matching in T_v results in Laplacian perfect state transfer in $\overset{n}{\uplus}X$ at $\frac{\pi}{2}$ between the end vertices of every edge inserted. Moreover, the resulting graph is periodic at $\frac{\pi}{2}$ at all vertices in T_u that are not incident to the newly added edges.*

By Theorem 8.9.1, the addition of a matching in $\overset{n}{\uplus}X$ as described above works as long as the vertices in the matching belong to a set twins. Thus, if v and u are false twins in X, then $T_v \cup T_u$ is a false twin set in $\overset{n}{\uplus}X$ by Proposition 8.1.1, and so the conclusion in Theorem 8.9.2 still works if we add a matching in $T_v \cup T_u$.

Corollary 8.9.3. *Let $n \equiv 0$ (mod 4). If u and v are false twins in X with $\Phi_{\mathbf{e}_v}(X) \subset \mathbb{Z}$, then the addition of a matching in $T_v \cup T_u$ results in PST in $\overset{n}{\uplus}X$ at $\frac{\pi}{2}$ between the end vertices of every edge inserted. Moreover, the resulting graph is periodic at all vertices in T_v that are not incident to the newly added edges with period $\frac{\pi}{2}$.*

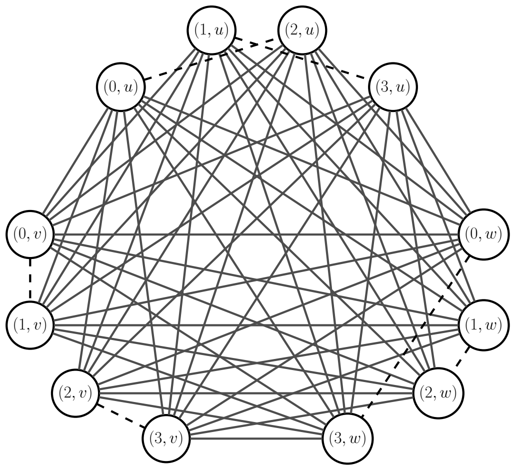

Figure 8.3: PST in $\overset{4}{\uplus} K_3$ between the end vertices of dashed edges.

In general, one may begin with any graph X such that $\operatorname{spec}(L(X)) \subseteq \mathbb{Z}$, and apply Theorem 8.9.1 repeatedly to $\overset{n}{\uplus} X$ where $n \equiv 0 \pmod 4$ to construct new graphs having PST.

Next, combining Theorem 8.9.2 and Corollary 8.9.3 yields the following result.

Corollary 8.9.4. *Let $n \equiv 0$ (mod 4) and u be a vertex in X with $\Phi_{\mathbf{e}_u}(X) \subset \mathbb{Z}$.*

1. *If u has no false twins in X, then the addition of a perfect matching in T_u results in PST in $\overset{n}{\uplus} X$ at $\frac{\pi}{2}$ between the end vertices of every edge inserted.*

2. *If u has a false twin v in X, then the addition of a perfect matching in $T_u \cup T_v$ results in PST in $\overset{n}{\uplus} X$ at $\frac{\pi}{2}$ between the end vertices of every edge inserted.*

We demonstrate Theorem 8.9.2 and Corollary 8.9.4(1) in the following examples.

Example 8.9.5. Suppose K_3 has vertices u, v, w. Here $\overset{4}{\uplus} K_3$ can be realised as a complete 3-partite graph as shown in Figure 8.3 with partite sets T_u, T_v and T_w. As $\operatorname{spec}(L(K_3)) \subseteq \mathbb{Z}$, the addition of any set of pairwise non-adjacent edges in T_u, T_v and T_w results in PST in $\overset{4}{\uplus} K_3$ at $\frac{\pi}{2}$ between the end vertices of every edge inserted.

We end this section with an illustration of Theorem 8.9.2 and Corollary 8.9.4(2).

Example 8.9.6. Suppose C_4 vertices has edges $\{a, b\}, \{b, c\}, \{c, d\}, \{d, a\}$. Note that $\{a, c\}$ and $\{b, d\}$ are pairs of false twins in C_4. Since $\operatorname{spec}(L(X)) \subseteq \mathbb{Z}$, addition of any set of pairwise non-adjacent edges in $T_a \cup T_c$ and $T_b \cup T_d$ results in PST in $\overset{4}{\uplus} C_4$ at $\frac{\pi}{2}$ between the end vertices of every edge inserted, see Figure 8.4.

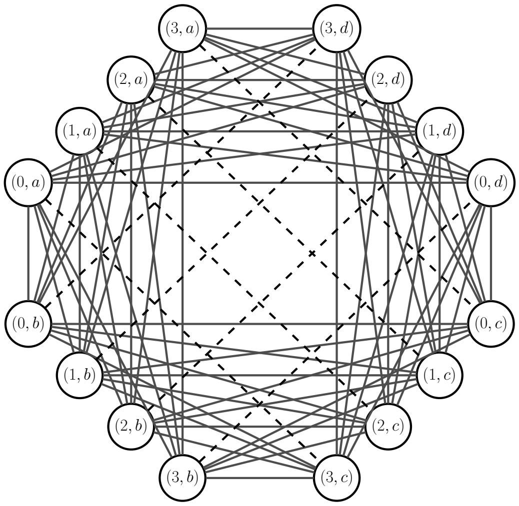

Figure 8.4: PST in $\overset{4}{\uplus}\, C_4$ between the end vertices of dashed edges.

9

s-pair state transfer

In this chapter, we deal with s-pair states. These are pure states of the form $\mathbf{e}_u + s\mathbf{e}_v$, where u and v are two vertices in X and $s \in \mathbb{C}\backslash\{0\}$. A (1)-pair state is called a plus state while a (-1)-pair state is called a pair state.

Physically speaking, an s-pair state $\mathbf{e}_u + s\mathbf{e}_v$ represents a pair of entangled qubits [64]. The parameter s may be viewed as a measure of the degree of entanglement of the qubits u and v in the s-pair state represented by $\mathbf{e}_u + s\mathbf{e}_v$. The closer $|s|$ is to 1, the closer the s-pair state $\mathbf{e}_u + s\mathbf{e}_v$ is to a maximally entangled state. Consequently, pair and plus states are maximally entangled. The *Bell states*, which are pure states in $\mathbb{C}^4$ of the form $\frac{1}{\sqrt{2}}(\mathbf{e}_1 \pm \mathbf{e}_4)$, $\frac{1}{\sqrt{2}}(\mathbf{e}_2 \pm \mathbf{e}_3)$, are examples of pair and plus states. Given the interpretation of s-pair states, it follows that PST between from an s- to an r-pair state represents a mapping of entangled states to entangled states. In particular, perfect state transfer from an s- to an r-pair state with $|s| = |r|$ can be viewed as PST on entangled states that have the same degree of entanglement.

Chen first investigated perfect state transfer between *edge states*, which are pair and plus states that form edges in a graph relative to the Laplacian matrix [27]. Such a phenomenon is called *edge state transfer*. This was extended by Chen and Godsil to include pair and plus states that need not form edges in the graph [28]. Later on, Kim et al. developed the theory of s-pair state transfer to generate more examples of perfect state transfer between entangled states [64].

Our goal in this chapter is to establish the algebraic and combinatorial properties of strongly cospectral s-pair states, characterise s-pair state transfer in complete graphs, complete bipartite graphs, paths and distance-regular graphs, and provide constructions of s-pair states that admit perfect state transfer. This leads to new interesting families of graphs that admit s-pair state transfer.

This chapter is based on two joint projects of the author. One is completed in joint work with Dr. Bahman Ahmadi, Dr. Ada Chan, Dr. Sooyeong Kim, Dr. Stephen Kirkland, and Dr. Sarah Plosker [64], while the other one is on-going in joint work with Dr. Ada Chan, Dr. Sooyeong Kim, Dr. Stephen Kirkland, Dr. Sarah Plosker, and Dr. Xiaohong Zhang [24]. The results presented in this chapter are the contributions of the author to these joint projects.

The following definition is obtained from Definition 4.0.1 where the pure states involved are an s- and an r-pair state that have the same moduli. Throughout this chapter, we assume that $(s, r) \in \mathbb{C}^2\backslash\{(0, 0)\}$ and $a, b, \alpha, \beta \in V(X)$ such that $a \neq b$ and $\alpha \neq \beta$.

Definition 9.0.1. Suppose $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + r\mathbf{e}_\beta$ are linearly independent vectors in $\mathbb{C}^n$. There is *perfect state transfer* (PST) from an s-pair state $\mathbf{u}$ to an r-pair state $\boldsymbol{\mu}$ (in X relative to M) if there is a time $\tau > 0$ and a complex number γ called *phase factor* such that

$$U_M(\tau)\left(\frac{1}{\sqrt{1+|s|^2}}\right)\mathbf{u} = \gamma\left(\frac{1}{\sqrt{1+|r|^2}}\right)\boldsymbol{\mu}. \tag{9.0.1}$$

The minimum such $\tau > 0$ is called the *minimum PST time*. Additionally, if $r = s$, then we say that *s-pair state transfer* occurs from $\mathbf{u}$ to $\boldsymbol{\mu}$. Furthermore, if $r = s = 1$ (respectively, $r = s = -1$), then we say that *plus state transfer* (respectively, *pair state transfer*) occurs from $\mathbf{u}$ to $\boldsymbol{\mu}$.

Remark 9.0.2. From Remark 4.0.2, the definition of PST from $\mathbf{x}$ to $\mathbf{y}$ implies that $\|\mathbf{x}\| = \|\mathbf{y}\|$. Therefore, strictly speaking, PST does not occur from the pure state $\mathbf{e}_u + s\mathbf{e}_v$ to the pure state $\mathbf{e}_w + r\mathbf{e}_x$ when $|r| \neq |s|$. However, normalising these vectors yields pure states with the same Euclidean norms. We take this fact into account in Definition 9.0.1: an s- and an r-pair state admit PST if and only if their corresponding normalised vectors admit PST.

Remark 9.0.3. If $|r| = |s|$, then the constants $\frac{1}{\sqrt{1+|s|^2}}$ and $\frac{1}{\sqrt{1+|r|^2}}$ are equal, and may be omitted from (9.0.1). Additionally, if $|r| = 1$, then we may write (9.0.1) as

$$U_M(\tau)(\mathbf{e}_u + s\mathbf{e}_v) = r\gamma(\mathbf{e}_x + \overline{r}\mathbf{e}_w).$$

Thus, if $|r| = |s| = 1$, then perfect state transfer between an s- and r- pair state gives rise to perfect state transfer between an s- and $\overline{r}$- pair state.

Remark 9.0.4. Suppose the pure states $\alpha\mathbf{e}_u + \beta\mathbf{e}_v$ and $\delta\mathbf{e}_w + \eta\mathbf{e}_x$ admit PST, where $\alpha, \beta, \delta, \eta \in \mathbb{C}\backslash\{0\}$. By Definition 9.0.1, this means that there is a time τ and a unit complex number γ such that

$$U(\tau)(\alpha\mathbf{e}_u + \beta\mathbf{e}_v) = \gamma(\delta\mathbf{e}_w + \eta\mathbf{e}_x).$$

Observe that $|\alpha|^2 + |\beta|^2 = \|\alpha\mathbf{e}_u + \beta\mathbf{e}_v\|^2 = \|\delta\mathbf{e}_w + \eta\mathbf{e}_x\|^2 = |\delta|^2 + |\eta|^2$. Thus, if $s = \frac{\beta}{\alpha}$ and $r = \frac{\eta}{\delta}$, then we may write the above equation as

$$U_M(\tau)\left(\frac{1}{\sqrt{1+|s|^2}}\right)(\mathbf{e}_u + s\mathbf{e}_v) = \gamma\gamma'\left(\frac{1}{\sqrt{1+|r|^2}}\right)(\mathbf{e}_w + r\mathbf{e}_x),$$

where $\gamma' = \frac{\delta|\alpha|}{\alpha|\delta|}$. Thus, PST on pure states with two nonzero entries is equivalent to PST from an s-pair state to an r-pair state up to a phase factor.

9.1 Strong cospectrality

Since strong cospectrality is a requirement for perfect state transfer, it is necessary to explore the properties of s-pair states that are strongly cospectral.

The first property we establish is a relation that certain entries of the spectral idempotents of M need to satisfy in order for strong cospectrality to occur.

Lemma 9.1.1. *Let $r, s \in \mathbb{C}\backslash\{0\}$. If $\frac{1}{\sqrt{1+|s|^2}}(\mathbf{e}_a + s\mathbf{e}_b)$ and $\frac{1}{\sqrt{1+|r|^2}}(\mathbf{e}_\alpha + r\mathbf{e}_\beta)$ are strongly cospectral with respect to M, then for all $j \geq 1$,*

$$\frac{1+|r|^2}{1+|s|^2}\left(|s|^2(E_j)_{b,b} + 2\operatorname{Re}(s)(E_j)_{a,b} + (E_j)_{a,a}\right) = |r|^2(E_j)_{\beta,\beta} + 2\operatorname{Re}(r)(E_j)_{\alpha,\beta} + (E_j)_{\alpha,\alpha}. \tag{9.1.1}$$

Proof. If $\mathbf{u} = \frac{1}{\sqrt{1+|s|^2}}(\mathbf{e}_a + s\mathbf{e}_b)$ and $\boldsymbol{\mu} = \frac{1}{\sqrt{1+|r|^2}}(\mathbf{e}_\alpha + r\mathbf{e}_\beta)$ are strongly cospectral, then they are weakly cospectral by Theorem 3.5.7. Simplifying $\mathbf{u}^* E_j \mathbf{u} = \boldsymbol{\mu}^* E_j \boldsymbol{\mu}$ yields the desired equation in (9.1.1). □

As a consequence of Lemma 9.1.1, strong cospectrality between an s- and an r-pair state impose a relation on certain entries of all powers of M.

Theorem 9.1.2. *Let $r, s \in \mathbb{C}\backslash\{0\}$. If $\frac{1}{\sqrt{1+|s|^2}}(\mathbf{e}_a + s\mathbf{e}_b)$ and $\frac{1}{\sqrt{1+|r|^2}}(\mathbf{e}_\alpha + r\mathbf{e}_\beta)$ are strongly cospectral with respect to M, then the expressions*

$$\frac{1+|r|^2}{1+|s|^2}\left(|s|^2(M^h)_{b,b} + 2\operatorname{Re}(s)(M^h)_{a,b} + (M^h)_{a,a}\right) \tag{9.1.2}$$

and

$$|r|^2(M^h)_{\beta,\beta} + 2\operatorname{Re}(r)(M^h)_{\alpha,\beta} + (M^h)_{\alpha,\alpha}. \tag{9.1.3}$$

are equal for all integers $h \geq 0$.

Proof. Summing (9.1.1) across all powers of distinct eigenvalues of M yields the equality of the expressions in (9.1.2) and (9.1.3). □

Corollary 9.1.3. *Let* $r, s \in \mathbb{C}\backslash\{0\}$. *Suppose* $\frac{1}{\sqrt{1+|s|^2}}(\mathbf{e}_a + s\mathbf{e}_b)$ *and* $\frac{1}{\sqrt{1+|r|^2}}(\mathbf{e}_\alpha + r\mathbf{e}_\beta)$ *are strongly cospectral relative to* M. *If* M *is a nonnegative matrix and* $\{a, b, \alpha, \beta\}$ *are pairwise cospectral pairs of vertices, then* $\operatorname{Re}(s)$ *and* $\operatorname{Re}(r)$ *are either both positive, both negative, or both zero. In the case that* $\operatorname{Re}(s)$ *and* $\operatorname{Re}(r)$ *are both nonzero, then* $\operatorname{dist}(a, b) = \operatorname{dist}(\alpha, \beta)$.

Proof. Since $\{a, b, \alpha, \beta\}$ are pairwise cospectral, we have

$$(M^h)_{a,a} = (M^h)_{b,b} = (M^h)_{\alpha,\alpha} = (M^h)_{\beta,\beta}$$

for all integers $h \geq 0$. Combining this with Theorem 9.1.2 yields

$$(1 + |r|^2)\operatorname{Re}(s)(M^h)_{a,b} = (1 + |s|^2)\operatorname{Re}(r)(M^h)_{\alpha,\beta}.$$

Since M is an irreducible nonnegative matrix, $(M^h)_{a,b} > 0$ for some h. Thus, $\operatorname{Re}(s)$ and $\operatorname{Re}(r)$ have the same signs. Moreover, if $\operatorname{Re}(s)$ and $\operatorname{Re}(r)$ are nonzero, then the above equation implies that $(M^h)_{a,b} = 0$ if and only if $(M^h)_{\alpha,\beta} = 0$, which implies that $\operatorname{dist}(a, b) = \operatorname{dist}(\alpha, \beta)$. □

9.2 When $r \in \{s, -s, \overline{s}\}$

Taking $r \in \{s, -s, \overline{s}\}$ in Theorem 9.1.2 yields the following result.

Theorem 9.2.1. *Let* $s \in \mathbb{C}\backslash\{0\}$. *If* $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ *and* $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ *are strongly cospectral with respect to* M, *then for all integers* $h \geq 0$,

$$|s|^2\left((M^h)_{b,b} - (M^h)_{\beta,\beta}\right) + 2\operatorname{Re}(s)\left((M^h)_{a,b} - (M^h)_{\alpha,\beta}\right) + (M^h)_{a,a} - (M^h)_{\alpha,\alpha} = 0. \tag{9.2.1}$$

If we replace $\boldsymbol{\mu}$ *by* $\mathbf{e}_\alpha + \overline{s}\mathbf{e}_\beta$, *then (9.2.1) still holds. Furthermore, if we replace* $\boldsymbol{\mu}$ *by* $\mathbf{e}_\alpha - s\mathbf{e}_\beta$, *then (9.2.1) holds with* $(M^h)_{a,b} - (M^h)_{\alpha,\beta}$ *replaced by* $(M^h)_{a,b} + (M^h)_{\alpha,\beta}$.

Corollary 9.2.2. *Let $s \in \mathbb{C}\backslash\{0\}$ and M be a nonnegative matrix. Suppose $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha - s\mathbf{e}_\beta$ are strongly cospectral with respect to M. If one of the conditions below hold, then s is purely imaginary.*

1. *$a = \alpha$ and $b = \beta$.*
2. *$a = \alpha$ and $\{b, \beta\}$ is a cospectral pair.*
3. *$b = \beta$ and $\{a, \alpha\}$ is a cospectral pair of vertices.*
4. *$\{a, \alpha\}$ and $\{b, \beta\}$ are cospectral pairs of vertices of vertices.*

Proof. This is immediate from Corollary 9.1.3 with $r = -s$. □

Proposition 9.2.3. *Let $s \in \mathbb{C}\backslash\{0\}$. Suppose M has constant row sum λ, and λ is a simple eigenvalue of M. If $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha - s\mathbf{e}_\beta$ are strongly cospectral, then s is purely imaginary and $E_\lambda \mathbf{u} = (\frac{1+s}{1-s})E_\lambda \boldsymbol{\mu}$.*

Proof. By assumption, we have $E_\lambda = \frac{1}{m}J_m$. Thus, $E_\lambda \mathbf{u} = \zeta E_\lambda \boldsymbol{\mu}$ if and only if $\zeta = \frac{1+s}{1-s}$. Now, $|\zeta| = 1$ if and only if $\mathrm{Re}(s) = 0$, and so s is purely imaginary. □

We obtain the following by applying Theorem 9.2.1 with $h = 1$.

Corollary 9.2.4. *Let $s \in \mathbb{C}\backslash\mathbb{R}$ with $\mathrm{Re}(s) \neq 0$. If $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha - s\mathbf{e}_\beta$ are strongly cospectral relative to A, then a and b (as well as α and β) are non-adjacent vertices in X.*

Theorem 9.2.5. *Let $s \in \mathbb{C}\backslash\{0\}$ with $\mathrm{Re}(s) \neq 0$. For any connected weighted graph X, the following hold for $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha - s\mathbf{e}_\beta$.*

1. *If $M = A$, then $\mathbf{u}$ and $\boldsymbol{\mu}$ are not strongly cospectral in X whenever one of the four conditions in Corollary 9.2.2 holds.*
2. *If (i) $M = L$, or (ii) $M = A$ and X is regular, then $\mathbf{u}$ and $\boldsymbol{\mu}$ are not strongly cospectral in X.*

Proof. Corollary 9.2.2 and Proposition 9.2.3 yield 1 and 2, respectively. □

If the parameter s in Theorem 9.2.1 is purely imaginary, then we can say more.

Corollary 9.2.6. *Let $f \in \mathbb{R}\backslash\{0\}$. If $\mathbf{u} = \mathbf{e}_a + \mathrm{i}f\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha \pm \mathrm{i}f\mathbf{e}_\beta$ are strongly cospectral relative to M, then the following hold.*

1. *The following are equivalent.*

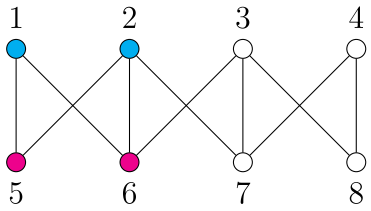

Figure 9.1: A counter-example to the conclusion of Proposition 9.2.7, where $a, b \in B_1$ with $a = 1, b = 2$

(a) Either $b = \beta$, or $\{b, \beta\}$ is a cospectral pair of vertices.

(b) Either $a = \alpha$, or $\{a, \alpha\}$ is a cospectral pair.

2. If $b \neq \beta$ and $\{b, \beta\}$ is not a cospectral pair of vertices, then for all integers $h \geq 0$, we have $f^2((M^h)_{b,b} - (M^h)_{\beta,\beta}) = (M^h)_{\alpha,\alpha} - (M^h)_{a,a}$. Additionally, if $M \in \{A, L\}$, then $f^2(\deg b - \deg \beta) = \deg \alpha - \deg a$.

Proof. Taking $s = \mathrm{i}f$ in Theorem 9.2.1 yields 1 and 2. □

Theorem 8.3 of [28] relates Laplacian perfect pair state transfer to perfect plus state transfer with respect to Q for bipartite graphs. In the following proposition, we give a similar result for strong cospectrality of s-pair states in bipartite graphs.

Proposition 9.2.7. *Let $s \in \mathbb{C} \backslash \{0\}$ and X be a bipartite graph with bipartition B_1 and B_2. Let $a, \alpha \in B_1$ and $b, \beta \in B_2$. Then the s-pair states $(\mathbf{e}_a + s\mathbf{e}_b)$ and $(\mathbf{e}_\alpha + s\mathbf{e}_\beta)$ are strongly cospectral with respect to Q if and only if $(\mathbf{e}_a - s\mathbf{e}_b)$ and $(\mathbf{e}_\alpha - s\mathbf{e}_\beta)$ are strongly cospectral with respect to L.*

Proof. For a weighted bipartite graph X, the matrix

$$P_{v,v} = \begin{cases} 1, & \text{if } v \in B_1, \\ -1, & \text{if } v \in B_2. \end{cases}$$

satisfies

$$Q = PLP \quad \text{and} \quad P(\mathbf{e}_a \pm s\mathbf{e}_b) = \mathbf{e}_a \mp s\mathbf{e}_b.$$

Hence, λ is an eigenvalue of L with associated eigenvector $\mathbf{w}$ if and only if λ is an eigenvalue of Q with associated eigenvector $P\mathbf{w}$. This implies that if E_λ is a spectral idempotent for L, then $F_\lambda = PE_\lambda P$ is a spectral idempotent for Q. Hence, if $F_\lambda(\mathbf{e}_a + s\mathbf{e}_b) = \zeta_\lambda F_\lambda(\mathbf{e}_\alpha + s\mathbf{e}_\beta)$ for some unit complex number z_λ, then we get

$E_\lambda P(\mathbf{e}_a + s\mathbf{e}_b) = \zeta_\lambda E_\lambda P(\mathbf{e}_\alpha + s\mathbf{e}_\beta)$, or equivalently, $E_\lambda(\mathbf{e}_a - s\mathbf{e}_b) = \zeta_\lambda E_\lambda P(\mathbf{e}_\alpha - s\mathbf{e}_\beta)$. This proves the forward direction. The converse follows similarly. $\square$

Proposition 9.2.7 does not necessarily hold for some values of s whenever $a, b \in B_1$. In Figure 9.1, we have $1, 2 \in B_1$, $5, 6 \in B_2$ and one checks that the states $\mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{e}_5 + \mathbf{e}_6$ are strongly cospectral in X relative to Q. However, $\mathbf{e}_1 - \mathbf{e}_2$ and $\mathbf{e}_5 - \mathbf{e}_6$ are not strongly cospectral in X relative to L. To see this, note that X is bipartite and $\lambda = 2$ is an eigenvalue of L and Q with an orthogonal set of eigenvectors given by

$$\{\mathbf{w}_1, \mathbf{w}_2\} := \{[1, -1, 0, 0, 0, 0, 1, -1]^T, [0, 0, 1, -1, 1, -1, 0, 0]^T\}$$

that works for both L and Q. This yields

$$E_\lambda(\mathbf{e}_1 - \mathbf{e}_2) = \frac{1}{2}(\mathbf{w}_1\mathbf{w}_1^T + \mathbf{w}_2\mathbf{w}_2^T)(\mathbf{e}_1 - \mathbf{e}_2) = \mathbf{w}_1.$$

Similarly, $E_\lambda(\mathbf{e}_5 - \mathbf{e}_6) = \mathbf{w}_2$, and so $E_\lambda(\mathbf{e}_1 - \mathbf{e}_2) \neq \zeta_\lambda E_\lambda(\mathbf{e}_5 - \mathbf{e}_6)$ for any unit $z_\lambda \in \mathbb{C}$. That is, $\mathbf{e}_1 - \mathbf{e}_2$ and $\mathbf{e}_5 - \mathbf{e}_6$ are not strongly cospectral relative to Q and L.

The next result states that strong cospectrality on s-pair states respects the symmetries of the graph. It is a special case of Lemma 3.5.10.

Proposition 9.2.8. *Let* $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ *and* $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ *be strongly cospectral s-pair states in X. If $s \neq 1$ then any automorphism of X that fixes (a, b) also fixes (α, β). If $s = 1$ then any automorphism of X that fixes $\{a, b\}$ also fixes $\{\alpha, \beta\}$.*

9.3 When s is real

In this section, we further investigate strongly cospectral s-pair states when s is real.

In an unweighted graph X, denote the number of common neighbours of two vertices a and b by $c_{ab} = (A^2)_{a,b}$. If $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$, then taking $M = A$ and $h = 2$ in (9.2.1) gives us

$$|s|^2 (\deg b - \deg \beta) + 2\operatorname{Re}(s)\,(c_{ab} - c_{\alpha\beta}) + \deg a - \deg \alpha = 0. \tag{9.3.1}$$

If we replace $\mathbf{u}$ by $\mathbf{e}_\alpha - s\mathbf{e}_\beta$, then (9.3.1) holds with $c_{ab} - c_{\alpha\beta}$ replaced by $c_{ab} + c_{\alpha\beta}$. From this, we get the following corollary which gives the precise value for s in terms of degrees and the number of common neighbours of the vertices involved whenever $\mathbf{e}_a + s\mathbf{e}_b$ and $\mathbf{e}_\alpha + s\mathbf{e}_\beta$ are strongly cospectral relative to A.

Corollary 9.3.1. *Let $s \in \mathbb{C}\backslash\{0\}$ and X be an unweighted graph. Suppose $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ are strongly cospectral relative to A.*

1. *Suppose $\deg b = \deg \beta$. If $\operatorname{Re}(s) = 0$ or $c_{ab} - c_{\alpha\beta} = 0$, then $\deg a = \deg \alpha$. Otherwise, $\operatorname{Re}(s) = \frac{\deg \alpha - \deg a}{2\left(c_{ab} - c_{\alpha\beta}\right)} \neq 0$.*

2. *Suppose $\deg b \neq \deg \beta$ and $s \in \mathbb{R}\backslash\{0\}$. If $\deg \alpha = \deg a$, then $s = -\frac{2(c_{ab} - c_{\alpha\beta})}{\deg b - \deg \beta}$. Otherwise,*

$$s = \frac{-(c_{ab} - c_{\alpha\beta}) \pm \sqrt{(c_{ab} - c_{\alpha\beta})^2 + (\deg b - \deg \beta)(\deg \alpha - \deg a)}}{\deg b - \deg \beta}.$$

If we replace $\mathbf{u}$ by $\mathbf{e}_\alpha - s\mathbf{e}_\beta$, then 1 and 2 holds with $c_{ab} - c_{\alpha\beta}$ replaced by $c_{ab} + c_{\alpha\beta}$.

Meanwhile, if $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$, then taking $M = L$ and $h = 1$ in (9.2.1) gives us

$$|s|^2 (\deg b - \deg \beta) - 2 \operatorname{Re}(s) \left((A)_{a,b} - (A)_{\alpha,\beta}\right) + \deg a - \deg \alpha = 0.$$

This yields an analogue of Corollary 9.3.1 relative to L.

Corollary 9.3.2. *Let $s \in \mathbb{C}\backslash\{0\}$. Suppose $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ are strongly cospectral relative to L.*

1. *Suppose $\deg b = \deg \beta$. If $\operatorname{Re}(s) = 0$ or $(A)_{a,b} - (A)_{\alpha,\beta} = 0$, then $\deg a = \deg \alpha$. Otherwise, $\operatorname{Re}(s) = \frac{\deg a - \deg \alpha}{2\left((A)_{a,b} - (A)_{\alpha,\beta}\right)} \neq 0$. Additionally, if X is unweighted and $\operatorname{Re}(s) \neq 0$, then $\operatorname{Re}(s) = \pm \frac{\deg a - \deg \alpha}{2}$ whenever exactly one of the pairs $\{a, b\}$ and $\{\alpha, \beta\}$ are adjacent, and $\deg a = \deg \alpha$ otherwise.*

2. *Suppose $\deg b \neq \deg \beta$ and $s \in \mathbb{R}\backslash\{0\}$. If $\deg \alpha = \deg a$, then $s = \frac{2((A)_{a,b} - (A)_{\alpha,\beta})}{\deg b - \deg \beta}$. Otherwise,*

$$s = \frac{((A)_{a,b} - (A)_{\alpha,\beta}) \pm \sqrt{((A)_{a,b} - (A)_{\alpha,\beta})^2 + (\deg b - \deg \beta)(\deg \alpha - \deg a)}}{\deg b - \deg \beta}.$$

If we replace $\mathbf{u}$ by $\mathbf{e}_\alpha - s\mathbf{e}_\beta$, then 1 and 2 holds with $(A)_{a,b} - (A)_{\alpha,\beta}$ replaced by $(A)_{a,b} + (A)_{\alpha,\beta}$.

In what follows, we let $d_{\max}$ denote the maximum degree of X. Using Corollaries 9.3.1 and 9.3.2, we provide bounds for the values of $s \in \mathbb{R}\backslash\{0\}$ whenever $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha \pm s\mathbf{e}_\beta$ are strongly cospectral relative to A and L.

Corollary 9.3.3. *Let* $s \in \mathbb{R}\backslash\{0\}$*,* X *be an unweighted graph and* $M \in \{A, L\}$*. Suppose* $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ *and* $\boldsymbol{\mu} = \mathbf{e}_\alpha \pm s\mathbf{e}_\beta$ *are strongly cospectral relative to* M*. Define*

$$\delta := \begin{cases} |c_{ab} - c_{\alpha\beta}| & \text{if } \boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta \\ c_{ab} + c_{\alpha\beta} & \text{otherwise} \end{cases}$$

when $M = A$*, and*

$$\delta := \begin{cases} 1 & \text{if } \boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta \\ 2 & \text{otherwise} \end{cases}$$

when $M = L$*. If* $\deg b \neq \deg \beta$*, then*

$$|s| \leq \begin{cases} 2\delta, & \text{if } \deg \alpha = \deg a \\ \delta + \sqrt{\delta^2 + d_{\max} - 1} & \text{otherwise.} \end{cases}$$

Proof. Let $\deg b \neq \deg \beta$. The result for the case $\deg \alpha = \deg a$ is immediate from the second statements of Corollaries 9.3.1 and 9.3.2. Now, let $\deg \alpha \neq \deg a$. We only prove the case when $M = A$, as the proof of the case $M = L$ is similar. Let $x = \deg b - \deg \beta$, $y = \deg \alpha - \deg a$ and $z = c_{ab} - c_{\alpha\beta}$. Note that $|y| \leq d_{\max} - 1$. Applying Corollary 9.3.1(2) with $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ yields

$$s_{\pm} = \frac{-z \pm \sqrt{z^2 + xy}}{x}.$$

Differentiating $s_{\pm}$ with respect to x gives us

$$\frac{d}{dx}s^{+} = \frac{-2z^2 - xy + 2z\sqrt{z^2 + xy}}{2x^2\sqrt{z^2 + xy}} \quad \text{and} \quad \frac{d}{dx}s^{-} = \frac{2z^2 + xy + 2z\sqrt{z^2 + xy}}{2x^2\sqrt{z^2 + xy}}.$$

First, let $x, y > 0$ so that $s_+ > 0$, $s_- < 0$, $\frac{d}{dx}s^{+} < 0$ and $\frac{d}{dx}s^{-} > 0$. This means that the maximum for s_+ and the minimum for s_- are attained when $x = 1$. In this case, we obtain

$$s_+ = -z + \sqrt{z^2 + y} \leq -(c_{ab} - c_{\alpha\beta}) + \sqrt{(c_{ab} - c_{\alpha\beta})^2 + d_{\max} - 1} \leq \delta + \sqrt{\delta^2 + d_{\max} - 1} \tag{9.3.2}$$

and

$$s_- = -z - \sqrt{z^2 + y} \geq -(c_{ab} - c_{\alpha\beta}) - \sqrt{(c_{ab} - c_{\alpha\beta})^2 + d_{\max} - 1} \geq -\delta - \sqrt{\delta^2 + d_{\max} - 1}. \tag{9.3.3}$$

Now, if $x > 0$ and $y < 0$, then $s_- < s_+ < 0$. One then checks that the upper bound for s_+ for this case is smaller than that of the previous case, while the lower bound for s_- remains the same. Combining (9.3.2) and (9.3.3) yields $|s| \leq \delta + \sqrt{\delta^2 + d_{\max} - 1}$. The case when $x < 0$ can be proven using the same argument. Furthermore, the case when $M = L$ can be proven similarly using Corollary 9.3.2(2). $\square$

9.4 Periodicity

We continue unravelling the properties of s-pair states, this time in relation to eigenvalue supports and periodicity. The following result gives a lower bound on the size of the eigenvalue support of an s-pair state.

Proposition 9.4.1. *Let $s \in \mathbb{C}\backslash\{0\}$ and M be a nonnegative matrix. If $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ is not a fixed state then*

$$|\Phi_{\mathbf{u}}| \geq \left\lceil \frac{\text{dist}(a,b)}{2} \right\rceil .$$

Proof. Let r be the covering radius of $\mathbf{u}$. Then $r \geq \left\lfloor \frac{\text{dist}(a,b)}{2} \right\rfloor$ and so $r+1 \geq \left\lceil \frac{\text{dist}(a,b)}{2} \right\rceil$. Invoking Lemma 6.3.1, we get that $|\Phi_{\mathbf{u}}| \geq r+1 \geq \left\lceil \frac{\text{dist}(a,b)}{2} \right\rceil$ as desired. $\square$

Remark 9.4.2. Since Proposition 9.4.1 applies to the nonnegative matrix $M = d_{\max}I - L$, it also applies to L.

Remark 9.4.3. The lower bound in Proposition 9.4.1 is tight for some families of graphs. For example, if a, b are the end vertices of P_n with n even, then $\mathbf{e}_a$ and $\mathbf{e}_b$ are strongly cospectral relative to A with $\Phi^+_{\mathbf{e}_a,\mathbf{e}_b} = \{\mu_j : 1 \leq j \leq n \text{ odd}\}$ and $\Phi^-_{\mathbf{e}_a,\mathbf{e}_b} = \{\mu_j : 1 \leq j \leq n \text{ even}\}$, where each μ_j is given in Lemma 5.5.1. Since n is even and $|\Phi^+_{\mathbf{e}_a,\mathbf{e}_b}| = |\Phi^-_{\mathbf{e}_a,\mathbf{e}_b}| = \frac{n}{2}$, we see that

$$|\Phi_{\mathbf{e}_a \mp \mathbf{e}_b}| = |\Phi^{\pm}_{\mathbf{e}_a,\mathbf{e}_b}| = \frac{n}{2} = \left\lceil \frac{n-1}{2} \right\rceil = \left\lceil \frac{\text{dist}(a,b)}{2} \right\rceil .$$

Thus, the pair and the plus states $\mathbf{e}_a - \mathbf{e}_b$ and $\mathbf{e}_a + \mathbf{e}_b$ attain the lower bound in Proposition 9.4.1. The same argument together with Lemma 5.5.5 and Remark 9.4.2 yields the same result relative to L.

Corollary 9.4.4. *If $\Phi_{\mathbf{e}_a} \cup \Phi_{\mathbf{e}_b}$ satisfies the ratio condition then the s-pair state $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ is periodic for any $s \in \mathbb{R}\backslash\{0\}$.*

Proof. This result follows immediately from Theorem 3.7.3 and the fact that $\Phi_{\mathbf{u}} \subseteq \Phi_{\mathbf{e}_a} \cup \Phi_{\mathbf{e}_b}$. $\square$

Remark 9.4.5. If $\mathbf{e}_a$ and $\mathbf{e}_b$ are periodic at the same time and the same phase factor, i.e., $U(\tau)\mathbf{e}_a = \eta\mathbf{e}_a$ and $U(\tau)\mathbf{e}_b = \eta\mathbf{e}_b$, then

$$U(\tau)(\mathbf{e}_a + s\mathbf{e}_b) = \eta(\mathbf{e}_a + s\mathbf{e}_b)$$

and so $\mathbf{e}_a + s\mathbf{e}_b$ is periodic for any $s \in \mathbb{C}\backslash\{0\}$.

Proposition 9.4.6. *Let a and b be cospectral vertices in X and $s \in \mathbb{C}\backslash\{0\}$. If $\mathbf{e}_a + s\mathbf{e}_b$ is periodic at time τ, then either $s = \pm 1$ or both vertex states $\mathbf{e}_a$ and $\mathbf{e}_b$ are periodic at time τ.*

Proof. Suppose $U(\tau)(\mathbf{e}_a + s\mathbf{e}_b) = \eta(\mathbf{e}_a + s\mathbf{e}_b)$ for some phase factor γ. Then

$$\begin{cases} U(\tau)_{a,a} + sU(\tau)_{a,b} = \gamma \\ U(\tau)_{b,a} + sU(\tau)_{b,b} = s\gamma. \end{cases}$$

Since a and b are cospectral, Lemmas 3.4.3 yields $U(\tau)_{a,a} = U(\tau)_{b,b}$. Moreover, because $U(\tau)$ is symmetric, we have $U(\tau)_{a,b} = U(\tau)_{b,a}$. Thus, the above system of equations gives

$$(s^2 - 1)U(\tau)_{a,b} = 0.$$

Hence, either $s = \pm 1$, or $U(\tau)_{a,a} = U(\tau)_{b,b} = \gamma$. □

We complement Proposition 9.4.6 and Corollary 9.4.4 by illustrating an infinite family of graphs with periodic pair states but the associated vertex states are not.

Example 9.4.7. Let X be a conference graph on n vertices, where n is not a perfect square. That is, X is a strongly-regular graph whose multiplicities of the two eigenvalues (other than the valency) of the adjacency matrix are equal. Please see Section 9.8 for the definition of a strongly-regular graph.

Note that X is k-regular, where $k = (n-1)/2$. In this case,

$$\operatorname{spec}(A) = \left\{k, \frac{-1+\sqrt{n}}{2}, \frac{-1-\sqrt{n}}{2}\right\},$$

which does not satisfy the ratio condition. Since $\Phi_{\mathbf{e}_u} = \operatorname{spec}(A)$ for each vertex u of X, we conclude that X has no periodic vertices. Now, let $\mathbf{u} = \mathbf{e}_a - \mathbf{e}_b$. If we let $\lambda_1 = k$, then $E_{\lambda_1} = \frac{1}{n}J$, and so $E_{\lambda_1}\mathbf{u} = \mathbf{0}$. This implies that $\Phi_{\mathbf{u}} = \{(-1 \pm \sqrt{n})/2\}$, which satisfies the ratio condition. Invoking Theorem 3.7.3, the pair state $\mathbf{u}$ is periodic. This example also illustrates Proposition 9.4.6. Indeed, since X is a strongly-regular graph, it is a walk-regular graph, and so all pairs of vertices are cospectral by Remark 6.2.5. In this case, if an s-pair state $\mathbf{e}_a + s\mathbf{e}_b$ is periodic in X, then either $s = \pm 1$ or a, b are both periodic by Proposition 9.4.6. However, the latter condition does not hold, and because $\Phi_{\mathbf{e}_a+\mathbf{e}_b} = \operatorname{spec}(A)$, we know that $\mathbf{e}_a + \mathbf{e}_b$ is also not periodic. Thus, $s = -1$, in which case $\mathbf{u} = \mathbf{e}_u - \mathbf{e}_v$ is periodic in X.

We close this section with the following corollary.

Corollary 9.4.8. *Let X be a weighted walk-regular graph such that $\phi(A, t)$ has integer coefficients, and suppose perfect state transfer occurs between m-strongly cospectral s-pair states $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_u + s\mathbf{e}_v$ relative to A. If $\operatorname{spec}(A)\backslash\mathbb{Z} \neq \varnothing$ (equivalently, the quantum walk on A is not periodic), then $s \in \{\pm 1\}$.*

Proof. If PST occurs between m-strongly cospectral s-pair states $\mathbf{u}$ and $\boldsymbol{\mu}$, then they are periodic states by virtue of Theorem 4.2.3. Since X is a weighted walk-regular graph, $\phi(A, t)$ has integer coefficients and $\operatorname{spec}(A)\backslash\mathbb{Z} \neq \varnothing$, Corollary 3.7.16 implies that any vertex a of X is not periodic. Since X is walk-regular, any pair of vertices in X are cospectral by Remark 6.2.5, and so invoking Proposition 9.4.6 yields the desired conclusion. □

9.5 Complete graphs

We now move on to characterise s-pair states that admit PST in common families of graphs, starting with complete graphs.

Corollary 9.5.1. *Let $V(K_n) = \{1, \ldots, n\}$, $\mathbf{x} = \mathbf{e}_1 + s\mathbf{e}_2$ with $s \in \mathbb{C}\backslash\{0, -1\}$ and $\mathbf{y} \in \mathbb{C}^n$ be a vector that has two nonzero entries. Perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in K_n relative to A at time τ if and only one of the following conditions hold.*

1. *$n = 2$, $\mathbf{y} = \frac{e^{\mathrm{i}2\tau}+1+s(e^{\mathrm{i}2\tau}-1)}{2}\mathbf{e}_1 + \frac{e^{\mathrm{i}2\tau}-1+s(e^{\mathrm{i}2\tau}+1)}{2}\mathbf{e}_2$.*
2. *$n = 3$, $s = \frac{2+e^{\mathrm{i}3t}}{1-e^{\mathrm{i}3\tau}}$, and $\mathbf{y} = \mathbf{e}_3 + (s-1)\mathbf{e}_2$.*
3. *$n = 3$, $s = \frac{1-e^{\mathrm{i}3\tau}}{2+e^{\mathrm{i}3\tau}}$, and $\mathbf{y} = s\mathbf{e}_3 + (1-s)\mathbf{e}_1$.*
4. *$n = 4$, $s = 1$, $\mathbf{y} = \mathbf{e}_3 + \mathbf{e}_4$ and $\tau = \frac{\pi}{4}$.*

Proof. Let $\mathbf{x} = \mathbf{e}_1 + s\mathbf{e}_2$, where $s \in \mathbb{C}\backslash\{0\}$. From Theorem 5.2.1, PST occurs from $\mathbf{x}$ to $\mathbf{y}$ in K_n at time τ if and only if $s \neq \pm 1$ and

$$\mathbf{y} = (\mathbf{e}_1 + s\mathbf{e}_2) + \left(\frac{(e^{\mathrm{i}\tau n} - 1)(1+s))}{n}\right)\mathbf{1}.$$

Since $\mathbf{x}$ has two nonzero entries, $\mathbf{y}$ has at least three nonzero entries whenever $n \geq 5$. Thus, $n \in \{2,3,4\}$. Moreover, $e^{\mathrm{i}\tau n} \neq 1$ otherwise $\mathbf{x} = \mathbf{y}$ is periodic at τ.

If $n = 2$, then $\mathbf{y} = \frac{1}{2}\begin{bmatrix} e^{\mathrm{i}2\tau} + 1 + s(e^{\mathrm{i}2\tau} - 1) \\ e^{\mathrm{i}2\tau} - 1 + s(e^{\mathrm{i}2\tau} + 1) \end{bmatrix}$. If $n = 3$, then PST occurs from $\mathbf{x}$ to $\mathbf{y} = \mathbf{x} + \left(\frac{(e^{\mathrm{i}3\tau}-1)(1+s)}{3}\right)\mathbf{1}$ at time τ. Now, $\mathbf{y}$ has two nonzero entries if and only if either $1 + \left(\frac{(e^{\mathrm{i}3\tau}-1)(1+s)}{3}\right) = 0$ or $s + \left(\frac{(e^{\mathrm{i}3\tau}-1)(1+s)}{3}\right) = 0$. Equivalently, $s = \frac{2+e^{\mathrm{i}3\tau}}{1-e^{\mathrm{i}3\tau}}$ or $s = \frac{1-e^{\mathrm{i}3\tau}}{2+e^{\mathrm{i}3\tau}}$. In particular, if $s = \frac{2+e^{\mathrm{i}3\tau}}{1-e^{\mathrm{i}3\tau}}$, then PST occurs from $\mathbf{x}$ to $\mathbf{y} = \mathbf{e}_3 + (1-s)\mathbf{e}_2$. Meanwhile, if $s = \frac{1-e^{\mathrm{i}3\tau}}{2+e^{\mathrm{i}3\tau}}$, PST occurs from $\mathbf{x}$ to $\mathbf{y} = s\mathbf{e}_3 + (s-1)\mathbf{e}_1$. Finally, if $n = 4$, then $\mathbf{y}$ has two nonzero entries if and only if $1 + \left(\frac{(e^{\mathrm{i}4\tau}-1)(1+s)}{4}\right) = 0$ and $s + \left(\frac{(e^{\mathrm{i}4\tau}-1)(1+s)}{4}\right) = 0$. That is, $s = \frac{3+e^{\mathrm{i}4\tau}}{1-e^{\mathrm{i}4\tau}} = \frac{1-e^{\mathrm{i}4\tau}}{3+e^{\mathrm{i}4\tau}}$. Equivalently, $\tau = \frac{\pi}{4}$ and $s = 1$. In this case, PST occurs between $\mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{e}_3 + \mathbf{e}_4$ in K_4 at $\frac{\pi}{4}$. □

The following are immediate from Theorem 9.5.1.

Corollary 9.5.2. *If $n \geq 5$, then perfect state transfer does not occur in K_n from an s- to an r-pair state.*

Corollary 9.5.3. *Let $V(K_n) = \{1, \ldots, n\}$. Real s-pair state transfer occurs in K_n relative to A at time τ if and only if one of the following conditions holds.*

1. *$n = 2$, from $\mathbf{e}_1 + s\mathbf{e}_2$ to $\mathbf{e}_2 + s\mathbf{e}_1$ with $s \neq \pm 1$, and $\tau = \frac{\pi}{2}$.*
2. *$n = 3$, between the pairs $\{\mathbf{e}_1 + \frac{1}{2}\mathbf{e}_2, \mathbf{e}_3 + \frac{1}{2}\mathbf{e}_2\}$, $\{\mathbf{e}_1 + 2\mathbf{e}_2, \mathbf{e}_1 + 2\mathbf{e}_3\}$ and $\tau = \frac{\pi}{3}$.*
3. *$n = 4$, between $\mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{e}_3 + \mathbf{e}_4$, and $\tau = \frac{\pi}{4}$.*

Proof. Note that K_n is periodic with $\rho = \frac{2\pi}{n}$. Thus, the PST time of any real state is $\frac{\pi}{n}$. Combining this with Theorem 9.5.1 yields the result. □

9.6 Complete bipartite graphs

For complete bipartite graphs, we establish results analogous to Corollaries 9.5.1 and 9.5.3 relative to A and L. Since K_2 is dealt with, we only examine $K_{a,b}$ with $a + b \geq 3$. We start with the case when $M = A$.

Theorem 9.6.1. *Let $V(K_{a,b}) = B_1 \cup B_2$, where $|B_1| = a$. Suppose $\mathbf{x} = \mathbf{e}_u + s\mathbf{e}_v$ for some $s \in \mathbb{C}\backslash\{0\}$ and $\mathbf{y} \in \mathbb{C}^n$ is a vector with two nonzero entries. Perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $K_{a,b}$ relative to A at time τ if and only if one of the following conditions hold.*

1. *$u, v \in B_1$, $s \neq -1$ and one of the conditions below holds.*

(a) $a=4$, $s=1$, *and* $\mathbf{y}=\mathbf{e}_w+\mathbf{e}_x$ *where* $B_1=\{u,w,v,x\}$, *and* $\tau=\frac{\pi}{2\sqrt{b}}$.

(b) $a=2$, $b=1$, $s=\cot^2(\tau/\sqrt{2})$, *and* $\mathbf{y}=(s-1)\mathbf{e}_v+\frac{1+s}{\sqrt{2}}\mathrm{i}\sin(\tau\sqrt{2})\mathbf{e}_w$.

(c) $a=2$, $b=1$, $s=\sec(\tau\sqrt{2})-1$, *and* $\mathbf{y}=(1-s)\mathbf{e}_u+\frac{1+s}{\sqrt{2}}\mathrm{i}\sin(\tau\sqrt{2})\mathbf{e}_w$.

(d) $a=2$, $b=2$, $s=1$, *and* $\mathbf{y}=\mathbf{e}_w+\mathbf{e}_x$ *where* $B_2=\{w,x\}$, *and* $\tau=\frac{\pi}{2}$.

2. $u\in B_1$, $v\in B_2$ *and one of the conditions below hold.*

(a) $a=1$, $b=2$, $\mathbf{y}=\mathbf{e}_u+s\mathbf{e}_w$ *where* $B_2=\{v,w\}$, *and* $\tau=\frac{\pi}{\sqrt{2}}$.

(b) $a=1$, $s=\sqrt{b}\cot(\tau\sqrt{b}/2)\mathrm{i}$, *and* $\mathbf{y}=\mathbf{e}_u-s\mathbf{e}_v$.

(c) $a=b=2$, $\mathbf{y}=\mathbf{e}_w+s\mathbf{e}_x$ *where* $B_1=\{u,w\}$ *and* $B_2=\{v,x\}$, *and* $\tau=\frac{\pi}{2}$.

Moreover, the above statements hold if we interchange the roles of a and b, as well as B_1 and B_2.

Proof. First, suppose $u,v\in B_1$. Then $s\neq -1$, otherwise $\mathbf{x}$ is fixed. We invoke Theorem 5.3.1 with $\mathbf{x}_1=\mathbf{e}_u+s\mathbf{e}_v$ and $\mathbf{x}_2=\mathbf{0}$. Making use of (5.3.1) gives us

$$\mathbf{y}=\begin{bmatrix}\mathbf{e}_u+s\mathbf{e}_v+\frac{1+s}{a}(\mathrm{Re}(e^{\mathrm{i}\tau\sqrt{ab}})-1)\mathbf{1}_a\\ \frac{1+s}{\sqrt{ab}}\mathrm{i}\,\mathrm{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\mathbf{1}_b\end{bmatrix}.$$

If $e^{\mathrm{i}\tau\sqrt{ab}}\in\mathbb{R}$, then $\mathrm{Im}(e^{\mathrm{i}\tau\sqrt{ab}})=0$ and $\tau=\frac{\ell\pi}{\sqrt{ab}}$ for any integer ℓ. If ℓ is even, then $\mathbf{x}$ is periodic at time τ. Otherwise, $\mathbf{y}$ has two nonzero entries if and only if $s=1$ and $a=4$. In this case, PST occurs between $\mathbf{e}_u+\mathbf{e}_v$ and $\mathbf{e}_w+\mathbf{e}_x$ at $\frac{\pi}{2}$, where $B_1=\{u,w,v,x\}$. Hence, 1a holds. On the other hand, if $e^{\mathrm{i}\tau\sqrt{ab}}\notin\mathbb{R}$, then $\mathrm{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\neq 0$. In particular, if $b=1$, then

$$\mathbf{y}=\begin{bmatrix}\mathbf{e}_u+s\mathbf{e}_v+\frac{1+s}{a}(\cos(\tau\sqrt{a})-1)\mathbf{1}_a\\ \frac{1+s}{\sqrt{a}}\mathrm{i}\sin(\tau\sqrt{a})\end{bmatrix},$$

which has two nonzero entries if and only if $a=2$ and $\frac{1+s}{2}(\cos(\tau\sqrt{2})-1)\in\{-1,-s\}$. The latter yields the values

$$s=\frac{1+\cos(\tau\sqrt{2})}{1-\cos(\tau\sqrt{2})}=\cot^2(\tau/\sqrt{2})\quad\text{and}\quad s=\frac{1-\cos(\tau\sqrt{2})}{\cos(\tau\sqrt{2})}=\sec(\tau/\sqrt{2})-1,$$

and the vectors

$$\mathbf{y}=(s-1)\mathbf{e}_v+\frac{1+s}{\sqrt{a}}\mathrm{i}\sin(\tau\sqrt{a})\mathbf{e}_w\quad\text{and}\quad\mathbf{y}=(1-s)\mathbf{e}_u+\frac{1+s}{\sqrt{a}}\mathrm{i}\sin(\tau\sqrt{a})\mathbf{e}_w$$

respectively. This proves 1b and 1c. However, if $b \neq 1$, then $b = 2$ and $\mathbf{e}_u + s\mathbf{e}_v + \frac{1+s}{a}(\cos(\tau\sqrt{2a}) - 1)\mathbf{1} = 0$, which yields $a = 2$, $s = 1$, $\tau = \frac{\pi}{2}$ and $\mathbf{y} = -\mathrm{i}(\mathbf{e}_w + \mathbf{e}_x)$, where $B_2 = \{w, x\}$. Ignoring the phase factor, 1d holds.

Next, assume $u \in B_1$ and $v \in B_2$. We again invoke Theorem 5.3.1 with $\mathbf{x}_1 = \mathbf{e}_u$ and $\mathbf{x}_2 = s\mathbf{e}_v$. Then (5.3.1) once again gives us

$$\mathbf{y} = \begin{bmatrix} \mathbf{e}_u + \Big((\mathrm{Re}(e^{\mathrm{i}\tau\sqrt{ab}}) - 1)\frac{1}{a} + s\,\mathrm{i}\,\mathrm{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\frac{1}{\sqrt{ab}}\Big)\,\mathbf{1}_a \\ s\mathbf{e}_v + \Big(\mathrm{i}\,\mathrm{Im}(e^{\mathrm{i}\tau\sqrt{ab}})\frac{1}{\sqrt{ab}} + s(\mathrm{Re}(e^{\mathrm{i}\tau\sqrt{ab}}) - 1)\frac{1}{b}\Big)\,\mathbf{1}_b \end{bmatrix}. \tag{9.6.1}$$

Suppose $a = 1$. Note that $e^{\mathrm{i}\tau\sqrt{b}} \neq 1$, otherwise $\mathbf{x}$ is periodic at time τ. If $e^{\mathrm{i}\tau\sqrt{b}} = -1$, then $\mathbf{y} = \begin{bmatrix} -1 \\ s(\mathbf{e}_v - 2\frac{1}{b}\mathbf{1}) \end{bmatrix}$, which has two nonzero entries if and only if $b = 2$, in which case $\tau = \frac{\pi}{\sqrt{2}}$, $\mathbf{y} = -(\mathbf{e}_u + s\mathbf{e}_w)$ and $B_2 = \{v, w\}$. Ignoring the phase factor, this establishes 2a. Now, if $e^{\mathrm{i}\tau\sqrt{b}} \neq \pm 1$, then $\sin(\tau\sqrt{b}) \neq 0$. In this case, $\mathbf{y}$ has the form

$$\mathbf{y} = \begin{bmatrix} \cos(\tau\sqrt{b}) + s\,\mathrm{i}\sin(\tau\sqrt{b})\frac{1}{\sqrt{b}} \\ s\mathbf{e}_v + \Big(\mathrm{i}\sin(\tau\sqrt{b})\frac{1}{\sqrt{b}} + s(\cos(\tau\sqrt{b}) - 1)\frac{1}{b}\Big)\,\mathbf{1}_b \end{bmatrix}.$$

Since $\mathbf{y}$ has two non-zero entries and $\sin(\tau\sqrt{b}) \neq 0$, we get

$$\mathrm{i}\sin(\tau\sqrt{b})\frac{1}{\sqrt{b}} + s(\cos(\tau\sqrt{b}) - 1)\frac{1}{b} = 0.$$

Equivalently, $s = -\frac{\mathrm{i}\sqrt{b}\sin(\tau\sqrt{b})}{\cos(\tau\sqrt{b})-1} = \sqrt{b}\cot(\tau\sqrt{b}/2)\mathrm{i}$. This implies that

$$\cos(\tau\sqrt{b}) + \Big(\frac{-\mathrm{i}\sqrt{b}\sin(\tau\sqrt{b})}{\cos(\tau\sqrt{b}) - 1}\Big)\mathrm{i}\sin(\tau\sqrt{b})\frac{1}{\sqrt{b}} = \frac{\cos^2(\tau\sqrt{b}) - \cos(\tau\sqrt{b}) + \sin^2(\tau\sqrt{b})}{\cos(\tau\sqrt{b}) - 1} = -1$$

and so we may write $\mathbf{y} = -(\mathbf{e}_u - s\mathbf{e}_v)$. Ignoring the phase factor, we obtain 2b. Now, suppose $a \geq 2$. Again, note that $e^{\mathrm{i}\tau\sqrt{ab}} \neq 1$, otherwise $\mathbf{x}$ is periodic at time τ. If $e^{\mathrm{i}\tau\sqrt{ab}} = -1$, then (9.6.1) yields

$$\mathbf{y} = \begin{bmatrix} \mathbf{e}_u - \frac{2}{a}\mathbf{1}_a \\ s(\mathbf{e}_v - \frac{2}{b}\mathbf{1}_b) \end{bmatrix}.$$

If $\mathbf{y}$ has two nonzero entries then $a + b \leq 4$. The case $a = 1$ is already dealt with so we assume $a = b = 2$. Then $\mathbf{y} = -(\mathbf{e}_w + s\mathbf{e}_x)$ and $\tau = \frac{\pi}{2}$, where $B_1 = \{u, w\}$ and $B_2 = \{v, x\}$. Ignoring the phase factor, we get 2c.

Finally, by symmetry, the above cases hold if we interchange the roles of a and

b, as well as B_1 and B_2. $\square$

The following is immediate from Theorem 9.6.1.

Corollary 9.6.2. *Let $V(K_{a,b}) = B_1 \cup B_2$, where $|B_1| = a$. Real s-pair state transfer occurs in $K_{a,b}$ relative to A at time τ if and only if one of the following conditions hold.*

1. *$u, v \in B_1$, and one of the conditions below holds.*
   (a) *$a = 4$, $\mathbf{x} = \mathbf{e}_u + \mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_w + \mathbf{e}_x$ where $B_1 = \{u, w, v, x\}$, and $\tau = \frac{\pi}{2\sqrt{b}}$.*
   (b) *$a = 2$, $b = 2$, $\mathbf{x} = \mathbf{e}_u + \mathbf{e}_v$, and $\mathbf{y} = \mathbf{e}_w + \mathbf{e}_x$ where $B_2 = \{w, x\}$, and $\tau = \frac{\pi}{2}$.*
2. *$u \in B_1$, $v \in B_2$, $s \in \mathbb{R}\backslash\{0\}$ and one of the conditions below hold.*
   (a) *$a = 1$, $b = 2$, $\mathbf{x} = \mathbf{e}_u + s\mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_u + s\mathbf{e}_w$ where $B_2 = \{v, w\}$, and $\tau = \frac{\pi}{\sqrt{2}}$.*
   (b) *$a = b = 2$, $\mathbf{x} = \mathbf{e}_u + s\mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_w + s\mathbf{e}_x$ where $B_1 = \{u, w\}$, and $\tau = \frac{\pi}{2}$.*

Moreover, the above statements hold if we interchange the roles of a and b, as well as B_1 and B_2.

Taking $s = \pm 1$ in Corollary 9.6.2 yields the following result.

Corollary 9.6.3. *Pair state transfer occurs in $K_{m,n}$ relative to A if and only if either (i) $(m, n) \in \{(1, 2), (2, 1)\}$, between $\mathbf{e}_u - \mathbf{e}_w$ and $\mathbf{e}_u - \mathbf{e}_x$, where u is a degree two vertex, or (ii) $m = n = 2$, between $\mathbf{e}_u - \mathbf{e}_w$ and $\mathbf{e}_v - \mathbf{e}_x$, where $\{u, w\}$ and $\{v, x\}$ are non-incident edges.*

Corollary 9.6.4. *Plus state transfer occurs in $K_{m,n}$ relative to A if and only if either (i) one of the two conditions in Corollary 9.6.3 holds with the pair states turned into plus states, or (ii) $m = 4$ or $n = 4$, between $\mathbf{e}_u + \mathbf{e}_w$ and $\mathbf{e}_v + \mathbf{e}_x$, where $\{u, w, v, x\}$ is a bipartition of size four.*

Remark 9.6.5. Suppose X is unweighted, $M = A$, and $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha - s\mathbf{e}_\beta$ are strongly cospectral. From Corollary 9.3.3, if $s \in \mathbb{R}$, then $|s|$ bounded above in terms of the maximum degree $d_{\max}$ of X and the number of common neighbours of a, b, as well as α, β. However, we see in the setting of Theorem 9.6.1(2b) that, s is purely imaginary and $|s| \to \infty$ whenever $\tau \to \frac{2\pi}{\sqrt{b}}$. Thus, if we allow s to be complex, then s may have arbitrarily large modulus unlike the case when s is real (see Corollary 9.3.3). This example not only presents an infinite family of graphs where PST occurs from an s-pair state $\mathbf{u}$ and its complex conjugate $\boldsymbol{\mu} = \overline{\mathbf{u}}$, but also illustrates an infinite family that satisfies Corollary 9.2.2(1). It also implies that if $\mathrm{Re}(s) = 0$, and $\mathbf{u}, \boldsymbol{\mu}$ are strongly cospectral, then the pairs of vertices $\{a, b\}$ and $\{\alpha, \beta\}$ are allowed to be adjacent. This observation complements Corollary 9.2.4.

Next, we deal with the case $M = L$.

Theorem 9.6.6. *Let $V(K_{a,b}) = B_1 \cup B_2$, where B_1 and B_2 are disjoint and $|B_1| = a$. Suppose $\mathbf{x} = \mathbf{e}_u + s\mathbf{e}_v$ for some $s \in \mathbb{C}\backslash\{0\}$ and $\mathbf{y} \in \mathbb{C}^n$ is a vector with two nonzero entries. Perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ in $K_{a,b}$ relative to L at time τ if and only if one of the following conditions hold.*

1. *$u, v \in B_1$, $s \neq -1$ and one of the conditions below hold.*
   - *(a) $a = 2$, $b = 1$, $e^{\mathrm{i}\tau} + \frac{1+s}{6}(2 + e^{\mathrm{i}3\tau} - 3e^{\mathrm{i}\tau}) = 0$, $\mathbf{y} = (s-1)e^{\mathrm{i}\tau}\mathbf{e}_v + \frac{1+s}{3}(1 - e^{\mathrm{i}3\tau})\mathbf{e}_w$ where $B_2 = \{w\}$, and τ satisfies $e^{\mathrm{i}3\tau} \neq 1$.*
   - *(b) $a = 2$, $b = 1$, $se^{\mathrm{i}\tau} + \frac{1+s}{6}(2 + e^{\mathrm{i}3\tau} - 3e^{\mathrm{i}\tau}) = 0$, $\mathbf{y} = (1-s)e^{\mathrm{i}\tau}\mathbf{e}_u + \frac{1+s}{3}(1 - e^{\mathrm{i}3\tau})\mathbf{e}_w$ where $B_2 = \{w\}$, and τ satisfies $e^{\mathrm{i}3\tau} \neq 1$.*
   - *(c) $a = b = 2$, $\mathbf{y} = \mathbf{e}_w + \mathbf{e}_x$ where $B_2 = \{w, x\}$, and $\tau = \frac{\pi}{4}$.*
   - *(d) $a = 2$, $\mathbf{y} = e^{-\mathrm{i}2\tau}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{2}(1 - e^{-\mathrm{i}2\tau})\mathbf{1}_2$, $e^{-\mathrm{i}2\tau} = e^{\mathrm{i}b\tau} \notin \{1, \frac{s+1}{s-2}, \frac{s+1}{1-2s}\}$.*
   - *(e) $a = 3$, $\mathrm{Re}\, s = \frac{1}{2}$, $s \neq 2$, $\mathbf{y} = \frac{s^2-1}{s-2}\mathbf{e}_v - \frac{s+1}{s-2}\mathbf{e}_w$ where $B_1 = \{u, v, w\}$ and τ satisfies $e^{\mathrm{i}3\tau} = \frac{s-2}{s+1}$.*
   - *(f) $a = 3$, $(\mathrm{Re}\, s - 1)^2 + (\mathrm{Im}\, s)^2 = 1$, $s \neq \frac{1}{2}$, $\mathbf{y} = \frac{s^2-1}{2s-1}\mathbf{e}_v + \frac{s^2+s}{2s-1}\mathbf{e}_w$ where $B_1 = \{u, v, w\}$, and τ satisfies $e^{\mathrm{i}3\tau} = \frac{1-2s}{s+1}$.*
   - *(g) $a = 4$, $b = 4k$ for any odd k, $\mathbf{y} = \mathbf{e}_w + \mathbf{e}_x$ where $B_1 = \{u, v, w, x\}$ and $\tau = \frac{\pi}{4}$.*
2. *$u \in B_1$, $v \in B_2$ and one of the conditions below hold.*
   - *(a) $a = 1$, $b = 2$, $s = \frac{2(e^{\mathrm{i}3\tau}-1)}{2+e^{\mathrm{i}3\tau}+3e^{\mathrm{i}\tau}} \neq \frac{1+2e^{\mathrm{i}3\tau}}{e^{\mathrm{i}3\tau}-1}$ with $e^{\mathrm{i}3\tau} \neq 1$, and $\mathbf{y} = \frac{1}{3}((1 + 2e^{\mathrm{i}3\tau}) + s(1 - e^{\mathrm{i}3\tau}))\mathbf{e}_u - se^{\mathrm{i}\tau}\mathbf{e}_w$, where $B_2 = \{v, w\}$.*
   - *(b) $a = b = 2$, $\mathbf{y} = \mathbf{e}_w + s\mathbf{e}_x$, $s \in \mathbb{C}\backslash\{0\}$ and $\tau = \frac{\pi}{2}$.*
   - *(c) $a = 2$, $b \geq 3$ is odd, $s = \frac{b}{2}$, $\mathbf{y} = \mathbf{e}_w + s\mathbf{e}_v$ where $B_1 = \{u, w\}$, at $\tau = \pi$.*
   - *(d) $a = 2$, $b = 4k$ for any integer k, $\mathbf{y} = \mathbf{e}_w - \mathbf{e}_v$ where $B_1 = \{u, w\}$, and $\tau = \frac{\pi}{2}$.*

Moreover, the above statements hold if we interchange the roles of a and b, as well as B_1 and B_2.

Proof. Suppose $u, v \in B_1$ so that $a \geq 2$. Then $s \neq -1$, otherwise $\mathbf{x}$ is fixed. We invoke Theorem 5.3.2 with $\mathbf{x}_1 = \mathbf{e}_u + s\mathbf{e}_v$ and $\mathbf{x}_2 = \mathbf{0}$. From (5.3.2), we obtain

$$\mathbf{y} = \begin{bmatrix} e^{\mathrm{i}\tau b}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{an}(a + be^{\mathrm{i}\tau n} - ne^{\mathrm{i}\tau b})\mathbf{1}_a \\ \frac{1+s}{n}(1 - e^{\mathrm{i}\tau n})\mathbf{1}_b \end{bmatrix}.$$

We proceed with two cases.

Case 1. Suppose $e^{\mathrm{i}\tau n} \neq 1$. Then $\frac{1+s}{n}(1 - e^{\mathrm{i}\tau n})\mathbf{1}_b \neq \mathbf{0}$, and so $\mathbf{y}$ has two nonzero entries if and only if either (i) $b = 1$ and $e^{\mathrm{i}\tau}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{a}(a + e^{\mathrm{i}\tau(a+1)} - (a+1)e^{\mathrm{i}\tau})\mathbf{1}_a$ has one nonzero entry or (ii) $b = 2$ and $e^{\mathrm{i}2\tau}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{an}(a + 2e^{\mathrm{i}\tau n} - ne^{\mathrm{i}2\tau})\mathbf{1}_a = \mathbf{0}$ or. Suppose condition (i) holds. If $a \geq 4$, then $a + e^{\mathrm{i}\tau(a+1)} - (a+1)e^{\mathrm{i}\tau} = 0$, which in turn yields $e^{\mathrm{i}\tau} = 0$, a contradiction. Thus, $a \in \{2, 3\}$. If $a = 3$, then $\mathbf{y}$ has two nonzero entries if and only if $s = 1$ and $e^{\mathrm{i}\tau b} + \frac{1+s}{an}(a + be^{\mathrm{i}\tau n} - ne^{\mathrm{i}\tau b}) = 0$, where $b = 1$ and $n = 4$. These conditions yield $e^{i4\tau} = 1$, a contradiction. For the case $a = 2$, we get that either $e^{\mathrm{i}\tau} + \frac{1+s}{6}(2 + e^{\mathrm{i}3\tau} - 3e^{\mathrm{i}\tau}) = 0$ or $se^{\mathrm{i}\tau} + \frac{1+s}{6}(2 + e^{\mathrm{i}3\tau} - 3e^{\mathrm{i}\tau}) = 0$. The former yields $\mathbf{y} = (s-1)e^{\mathrm{i}\tau}\mathbf{e}_v + \frac{1+s}{3}(1 - e^{\mathrm{i}3\tau})\mathbf{e}_w$, while the latter yields $\mathbf{y} = (1-s)e^{\mathrm{i}\tau}\mathbf{e}_u + \frac{1+s}{3}(1 - e^{\mathrm{i}3\tau})\mathbf{e}_w$. This proves 1a and 1b. Now, suppose condition (ii) holds. If $a \geq 3$, then $a + 2e^{\mathrm{i}\tau n} - ne^{\mathrm{i}2\tau} = 0$, which implies that $\mathbf{e}_u + s\mathbf{e}_v = \mathbf{0}$, a contradiction. Since $a \geq 2$, we get that $a = 2$. In this case, $\mathbf{y}$ has two nonzero entries if and only if $s = 1$ and $\tau = \frac{\pi}{4}$. This establishes 1c.

Case 2. Suppose $e^{\mathrm{i}\tau n} = 1$. Then $\mathbf{y}$ has two nonzero entries if and only if

$$e^{\mathrm{i}\tau b}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{a}(1 - e^{\mathrm{i}\tau b})\mathbf{1}_a$$

has two nonzero entries, which can only happen if $a \in \{2, 3, 4\}$. If $e^{\mathrm{i}\tau b} = 1$, then $\mathbf{x}$ is periodic, and so we may assume that $e^{\mathrm{i}\tau b} \neq 1$. We have three subcases. First, suppose $a = 2$. Then $e^{\mathrm{i}\tau b}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{2}(1 - e^{\mathrm{i}\tau b})\mathbf{1}_2$ has two nonzero entries if and only if both $(1+s) + (2-s)e^{\mathrm{i}\tau b}$ or $(1+s) + (2s-1)e^{\mathrm{i}\tau b}$ are nonzero. Equivalently, $e^{\mathrm{i}\tau b} \neq \frac{s+1}{s-2}$ and $e^{\mathrm{i}\tau b} \neq \frac{s+1}{1-2s}$. Since $e^{\mathrm{i}\tau n} = 1$, this proves 1d. Next, suppose $a = 3$. Then $e^{\mathrm{i}\tau b}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{a}(1 - e^{\mathrm{i}\tau b})\mathbf{1}_3$ has two nonzero entries if and only if exactly one of $(1+s) + (2-s)e^{\mathrm{i}\tau b}$ or $(1+s) + (2s-1)e^{\mathrm{i}\tau b}$ is equal to 0. If $(1+s) + (2-s)e^{\mathrm{i}\tau b} = 0$, then $e^{\mathrm{i}\tau b} = \frac{s+1}{s-2}$, $\operatorname{Re} s = \frac{1}{2}$ and $s \neq 2$ (otherwise, $s = -1$). In this case, we obtain $\mathbf{y} = \frac{s^2-1}{s-2}\mathbf{e}_v - \frac{s+1}{s-2}\mathbf{e}_w$. Since $e^{\mathrm{i}\tau n} = 1$, this proves 1e. On the other hand, if $(1+s)+(2s-1)e^{\mathrm{i}\tau b} = 0$, then $e^{\mathrm{i}\tau b} = \frac{s+1}{1-2s}$, $(\operatorname{Re} s - 1)^2 + (\operatorname{Im} s)^2 = 1$ and $s \neq \frac{1}{2}$ (otherwise $s = -1$). In this case, we obtain $\mathbf{y} = \frac{s^2+s}{s-2}\mathbf{e}_v - \frac{s^2+s}{1-2s}\mathbf{e}_w$. Since $e^{\mathrm{i}\tau n} = 1$, 1f holds. For the last subcase, suppose that $a = 4$. Then $e^{\mathrm{i}\tau b}(\mathbf{e}_u + s\mathbf{e}_v) + \frac{1+s}{a}(1 - e^{\mathrm{i}\tau b})\mathbf{1}_a$ has two nonzero entries if and only if $(1+s)+(a-1-s)e^{\mathrm{i}\tau b} = 0$ and $(1+s)+(as-1-s)e^{\mathrm{i}\tau b} = 0$, which holds if and only if $s=1$, $a=4$ and $e^{\mathrm{i}\tau b}=-1$. Since $\mathbf{x}$ is a real vector in this case and $K_{a,b}$ is periodic with $\rho=\frac{2\pi}{\gcd(a,b)}$, the minimum PST time is $\tau=\frac{\pi}{\gcd(a,b)}$ by Corollary 6.1.1. Since $e^{\mathrm{i}\tau b}=-1$, it follows that $\nu_2(\gcd(a,b))=\nu_2(b)=\nu_2(a)=2$, and so $b=4k$ for some odd k, which in turn gives us PST between $\mathbf{x}$ and $\mathbf{y}=\mathbf{e}_w+\mathbf{e}_x$ at $\tau=\frac{\pi}{4}$, where $B_1\{u,v,w,x\}$. This establishes 1g.

Suppose $u\in B_1$ and $v\in B_2$. We again make use of Theorem 5.3.2 with $\mathbf{x}_1=\mathbf{e}_u$ and $\mathbf{x}_2=s\mathbf{e}_v$. From (5.3.2), we obtain

$$\mathbf{y}=\begin{bmatrix} e^{\mathrm{i}\tau b}\mathbf{e}_u+\left(\frac{1}{an}(a+be^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau b})+\frac{s}{n}(1-e^{\mathrm{i}\tau n})\right)\mathbf{1}_a \\ se^{\mathrm{i}\tau a}\mathbf{e}_v+\left(\frac{s}{bn}(b+ae^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau a})+\frac{1}{n}(1-e^{\mathrm{i}\tau n})\right)\mathbf{1}_b\end{bmatrix}. \tag{9.6.2}$$

First, suppose $a=1$ and $b\geq 2$. In this case, $\mathbf{y}$ has two nonzero entries if and only if either (i) the vector $se^{\mathrm{i}\tau}\mathbf{e}_v+\left(\frac{s}{bn}(b+e^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau})+\frac{1}{n}(1-e^{\mathrm{i}\tau n})\right)\mathbf{1}_b$ has two nonzero entries and $e^{\mathrm{i}\tau b}+\left(\frac{1}{n}(1+be^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau b})+\frac{s}{n}(1-e^{\mathrm{i}\tau n})\right)=0$, or (ii) the vector $se^{\mathrm{i}\tau}\mathbf{e}_v+\left(\frac{s}{bn}(b+e^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau})+\frac{1}{n}(1-e^{\mathrm{i}\tau n})\right)\mathbf{1}_b$ has one nonzero entry and $e^{\mathrm{i}\tau b}+\left(\frac{1}{n}(1+be^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau b})+\frac{s}{n}(1-e^{\mathrm{i}\tau n})\right)\neq 0$. Condition (i) is already dealt in the case that $u,v\in B_1$. Now, suppose condition (ii) holds so that $b=2$. Then we have $se^{\mathrm{i}\tau a}+\left(\frac{s}{bn}(b+ae^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau a})+\frac{1}{n}(1-e^{\mathrm{i}\tau n})\right)=0$. Equivalently, $s=\frac{2(e^{\mathrm{i}3\tau}-1)}{2+e^{\mathrm{i}3\tau}+3e^{\mathrm{i}\tau}}$, where $e^{\mathrm{i}3\tau}\neq 1$ otherwise $\mathbf{x}$ is periodic. Since $e^{\mathrm{i}\tau b}+\left(\frac{1}{n}(1+be^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau b})+\frac{s}{n}(1-e^{\mathrm{i}\tau n})\right)\neq 0$, we also have $s\neq\frac{1+2e^{\mathrm{i}3\tau}}{e^{\mathrm{i}3\tau}-1}$. In this case, $\mathbf{y}=\frac{1}{3}((1+2e^{\mathrm{i}3\tau})+s(1-e^{\mathrm{i}3\tau}))\mathbf{e}_u-se^{\mathrm{i}\tau}\mathbf{e}_w$, where $B_2=\{v,w\}$. Now, suppose that $a\geq 2$. If $\mathbf{y}$ has two nonzero entries then we have two cases: either (i) $a=b=2$, or (ii) $a=2$, $b\geq 3$ and $\frac{s}{bn}(b+ae^{\mathrm{i}\tau n}-ne^{\mathrm{i}\tau a})+\frac{1}{n}(1-e^{\mathrm{i}\tau n})=0$.

Case 1. Suppose $a=b=2$. If $e^{\mathrm{i}2\tau}=1$, then $\mathbf{x}$ is periodic at time τ. If $e^{\mathrm{i}2\tau}=-1$, then (9.6.2) yields $\mathbf{y}=-\begin{bmatrix}\mathbf{e}_u-\mathbf{1}_2\\ s(\mathbf{e}_v-\mathbf{1}_2)\end{bmatrix}$, and so there is PST from $\mathbf{x}$ to $\mathbf{y}=\mathbf{e}_w+s\mathbf{e}_x$ at time $\frac{\pi}{2}$ for all $s\in\mathbb{C}\backslash\{0\}$. Since $\mathbf{x}$ is periodic at time τ whenever $e^{\mathrm{i}2\tau}\neq\pm 1$. If $(1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau})+s(1-e^{\mathrm{i}4\tau})=0$ and $s(1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau})+(1-e^{\mathrm{i}4\tau})=0$, we get that $\mathbf{y}$ has two nonzero entries if and only if either (i) $(1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau})+s(1-e^{\mathrm{i}4\tau})=0$ and $s(1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau})+(1-e^{\mathrm{i}4\tau})=-4e^{\mathrm{i}2\tau}$ or (ii) $s(1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau})+(1-e^{\mathrm{i}4\tau})=0$ and $(1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau})+s(1-e^{\mathrm{i}4\tau})=-4e^{\mathrm{i}2\tau}$. In both cases, we get

$$s=\frac{1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau}}{e^{\mathrm{i}4\tau}-1}=\frac{1-e^{\mathrm{i}4\tau}}{1+e^{\mathrm{i}4\tau}-2e^{\mathrm{i}2\tau}}.$$

Equivalently, $e^{\mathrm{i}2\tau}=1$, a contradiction.

Case 2. Suppose $a=2$, $b\geq 3$ and $\frac{s}{b}(b+2e^{\mathrm{i}\tau(b+2)}-(b+2)e^{\mathrm{i}2\tau})+(1-e^{\mathrm{i}\tau(b+2)})=0$. Note that $e^{\mathrm{i}2\tau}$ and $e^{\mathrm{i}b\tau}$ are not equal to 1, otherwise $\mathbf{x}$ is periodic at time τ. If $(e^{\mathrm{i}2\tau},e^{\mathrm{i}b\tau})=(1,-1)$, then b is odd and $\tau=\pi$. In this case, we obtain $s=\frac{b}{2}$ and

(9.6.2) gives us $\mathbf{y} = \mathbf{e}_w + \frac{b}{2}\mathbf{e}_v$ up to a phase factor, where $B_1 = \{u, w\}$. This yields 2b. Next, if $(e^{\mathrm{i}2\tau}, e^{\mathrm{i}b\tau}) = (-1, 1)$, then $b \equiv 0 \pmod 4$ and $\tau = \pi/2$. In this case, we have $s = -1$ and (9.6.2) again yields $\mathbf{y} = \mathbf{e}_w - \mathbf{e}_v$ up to a phase factor. This proves 2c. Now, if $(e^{\mathrm{i}2\tau}, e^{\mathrm{i}b\tau}) = (-1, -1)$, then we obtain $s = 0$, a contradiction. Thus, this case does not happen. Finally, suppose $e^{\mathrm{i}2\tau} \neq \pm 1$ and $e^{\mathrm{i}b\tau} \neq \pm 1$. We may write

$$s = \frac{b(e^{\mathrm{i}\tau(b+2)} - 1)}{b + 2e^{\mathrm{i}\tau(b+2)} - (b+2)e^{\mathrm{i}2\tau}}.$$

Since $\mathbf{y}$ has two nonzero entries and is linearly independent with $\mathbf{x}$,

$$\frac{1}{an}(a + be^{\mathrm{i}\tau n} - ne^{\mathrm{i}\tau b}) + \frac{s}{n}(1 - e^{\mathrm{i}\tau n}) = -e^{\mathrm{i}\tau b}.$$

Equivalently,

$$s = -\frac{2 + be^{\mathrm{i}\tau(b+2)} + (b+2)e^{\mathrm{i}\tau b}}{2(1 - e^{\mathrm{i}\tau(b+2)})}.$$

Therefore,

$$s = \frac{b(e^{\mathrm{i}\tau(b+2)} - 1)}{b + 2e^{\mathrm{i}\tau(b+2)} - (b+2)e^{\mathrm{i}2\tau}} = -\frac{2 + be^{\mathrm{i}\tau(b+2)} + (b+2)e^{\mathrm{i}\tau b}}{2(1 - e^{\mathrm{i}\tau(b+2)})},$$

which holds if and only if $(e^{\mathrm{i}2\tau} + 1)(e^{\mathrm{i}b\tau} + 1) = 0$, a contradiction to the fact that $e^{\mathrm{i}2\tau} \neq \pm 1$ and $e^{\mathrm{i}b\tau} \neq \pm 1$. This completes the proof of Case 2.

Combining all cases above yields the desired conclusion. □

The next result is straightforward from Theorem 9.6.6

Corollary 9.6.7. *Let $V(K_{a,b}) = B_1 \cup B_2$, where $|B_1| = a$. Real (s, r)-pair state transfer occurs in $K_{a,b}$ relative to L at time τ if and only if one of the following conditions hold.*

1. *$u, v \in B_1$, $s \neq -1$ and one of the conditions below hold.*
   - *(a) $a = 2$, $b = 1$, $\mathbf{x} = \mathbf{e}_u + \frac{1}{2}\mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_w + \frac{1}{2}\mathbf{e}_v$, $B_2 = \{w\}$, and $\tau = \pi$.*
   - *(b) $a = 2$, $b = 1$, $\mathbf{x} = \mathbf{e}_u + 2\mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_w + 2\mathbf{e}_v$, $B_2 = \{w\}$, and $\tau = \pi$.*
   - *(c) $a = b = 2$, $\mathbf{y} = \mathbf{e}_w + \mathbf{e}_x$ where $B_2 = \{w, x\}$, and $\tau = \frac{\pi}{4}$.*
   - *(d) $a = 2$, $b = 4k + 2$ for any integer k, $\mathbf{y} = \mathbf{e}_u + s\mathbf{e}_v$, $\mathbf{y} = s\mathbf{e}_u + \mathbf{e}_v$ and $\tau = \frac{\pi}{2}$.*
   - *(e) $a = 3$, $\mathbf{x} = \mathbf{e}_u + \frac{1}{2}\mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_w + \frac{1}{2}\mathbf{e}_v$ where $B_1 = \{u, v, w\}$, and $\tau = \frac{\pi}{3}$.*
   - *(f) $a = 3$, $\mathbf{x} = \mathbf{e}_u + 2\mathbf{e}_v$, $\mathbf{y} = \mathbf{e}_v + 2\mathbf{e}_w$ where $B_1 = \{u, v, w\}$, and $\tau = \frac{\pi}{3}$.*

   (g) *$a=4$, $b=4k$ for any odd k, $\mathbf{y}=\mathbf{e}_w+\mathbf{e}_x$ where $B_1=\{u,v,w,x\}$ and $\tau=\frac{\pi}{4}$.*

2. *$u\in B_1$, $v\in B_2$ and one of the conditions below hold.*
   - (a) *$a=1$, $b=2$, $\mathbf{x}=\mathbf{e}_u+2\mathbf{e}_v$, $\mathbf{y}=\mathbf{e}_u+2\mathbf{e}_w$ where $B_2=\{v,w\}$ and $\tau=\pi$.*
   - (b) *$a=b=2$, $\mathbf{x}=\mathbf{e}_u+s\mathbf{e}_v$, $\mathbf{y}=\mathbf{e}_w+s\mathbf{e}_x$, $s\in\mathbb{R}\backslash\{0\}$ and $\tau=\frac{\pi}{2}$.*
   - (c) *$a=2$, $b\geq 3$ is odd, $\mathbf{x}=\mathbf{e}_u+\frac{b}{2}\mathbf{e}_v$, $\mathbf{y}=\mathbf{e}_w+\frac{b}{2}\mathbf{e}_v$ where $B_1=\{u,w\}$, and $\tau=\pi$.*
   - (d) *$a=2$, $b=4k$ for any integer k, $\mathbf{x}=\mathbf{e}_u-\mathbf{e}_v$, $\mathbf{y}=\mathbf{e}_w-\mathbf{e}_v$ where $B_1=\{u,w\}$, and $\tau=\frac{\pi}{2}$.*

Moreover, the above statements hold if we interchange the roles of a and b, as well as B_1 and B_2.

Taking $s=\pm1$ in Corollary 9.6.7 yields the following corollaries.

Corollary 9.6.8. *Laplacian pair perfect state transfer occurs in $K_{m,n}$ if and only if either (i) $m=n=2$, between $\mathbf{e}_u-\mathbf{e}_w$ and $\mathbf{e}_v-\mathbf{e}_x$, where $\{u,w\}$ and $\{v,x\}$ are non-incident edges, or (ii) $(m,n)\in\{(2,4k),(4k,2)\}$ for any integer $k\geq 1$. In particular, perfect state transfer occurs between $\mathbf{e}_u-\mathbf{e}_w$ and $\mathbf{e}_v-\mathbf{e}_w$ in $K_{2,4k}$, where $\{u,v\}$ is a partite set of size two and $w\in V(K_{m,n})\backslash\{u,v\}$.*

In [27], it was shown that $K_{2,4k}$ admits Laplacian pair PST. Thus, C_4 and $K_{2,4k}$ are the only complete bipartite graphs that admit pair PST by Corollary 9.6.8. For plus state transfer, we have the following result.

Corollary 9.6.9. *Plus perfect state transfer occurs in $K_{m,n}$ relative to L if and only if one of the following conditions hold.*

1. *$m=n=2$, between $\mathbf{e}_u+\mathbf{e}_v$ and $\mathbf{e}_w+\mathbf{e}_x$, where either (i) $\{u,v\}$ and $\{w,x\}$ are non-incident edges or (ii) $\{u,v\}$ and $\{w,x\}$ are the two partite sets.*
2. *$(m,n)\in\{(4,4k),(4k,4)\}$ for any odd k, between $\mathbf{e}_u+\mathbf{e}_v$ and $\mathbf{e}_w+\mathbf{e}_x$, where $\{u,w,v,x\}$ is a partite set of size four.*

Lastly, from Theorems 9.6.1 and 9.6.6, the following results are straightforward.

Corollary 9.6.10. *If $a,b\geq 5$, then perfect state transfer does not occur in $K_{a,b}$ from an s- to an r-pair state relative to A and L.*

9.7 Paths

In this section, we make use of our results in to characterise pair and plus state transfer in paths.

Corollary 9.7.1. *Pair perfect state transfer occurs in P_n relative to A if and only if $n \in \{3, 5, 7\}$.*

Proof. Suppose pair PST occurs in P_n between $\mathbf{e}_u - \mathbf{e}_w$ and $\mathbf{e}_v - \mathbf{e}_x$. Since $\{u, w\} \neq \{v, x\}$, we have $n \geq 3$. Consider the eigenvectors $\mathbf{z}_j$ of $A(P_n)$ in Lemma 5.5.1. We proceed with two cases.

Case 1. Let $|\Phi_{\mathbf{e}_u - \mathbf{e}_w}(A)| = 2$. That is, $\mathbf{e}_u - \mathbf{e}_w = a\mathbf{z}_j + b\mathbf{z}_k$ and $\mathbf{e}_v - \mathbf{e}_x = a\mathbf{z}_j - b\mathbf{z}_k$ with $j \neq k$. This implies that $\sin(\frac{j\ell\pi}{n+1}) = \sin(\frac{k\ell\pi}{n+1}) = 0$ for any $\ell \neq u, w, v, x$. Since $j \neq k$, we get $\ell \neq 1, 2$, so we may assume that $u = 1$ and either $v = 2$ or $w = 2$. By Lemma 6.3.1, if $|\Phi_{\mathbf{e}_1 - \mathbf{e}_w}(A)| = 2$, then the covering radius of $\mathbf{e}_1 - \mathbf{e}_w$ is one. Hence, $n = 3$ and $w = 2$ or $n \in \{4, 5\}$ and $w = n$. Using Lemma 3.5.10, one checks that $\mathbf{e}_1 - \mathbf{e}_4$ and $\mathbf{e}_2 - \mathbf{e}_3$ are not strongly cospectral in P_4, while PST occurs between $\mathbf{e}_1 - \mathbf{e}_2$ and $\mathbf{e}_3 - \mathbf{e}_2$ in P_3 at time $\frac{\pi}{\sqrt{2}}$, and between $\mathbf{e}_1 - \mathbf{e}_5$ and $\mathbf{e}_2 - \mathbf{e}_4$ in P_5 at time $\frac{\pi}{2}$.

Case 2. Let $|\Phi_{\mathbf{e}_u - \mathbf{e}_w}(A)| = 3$. By Theorem 6.4.6, $\mathbf{e}_u - \mathbf{e}_w = a\mathbf{z}_{\frac{n+1}{2}} + b\mathbf{z}_j + c\mathbf{z}_k$ and $\mathbf{e}_v - \mathbf{e}_x = \mathbf{v}_\pm$, where $\mathbf{v}_\pm = a\mathbf{z}_{\frac{n+1}{2}} - b\mathbf{z}_j - c\mathbf{z}_k$ and $j, k \neq \frac{n+1}{2}$. If $\mathbf{e}_v - \mathbf{e}_x = \mathbf{v}_+$, then $\mathbf{e}_u + \mathbf{e}_v - \mathbf{e}_w - \mathbf{e}_x = 2a[1, 0, -1, 0, 1, \ldots]^T$. This holds if and only if $u, v \in \{1, 5\}$, $w, x \in \{3, 7\}$, $n = 7$ and $a = \frac{1}{2}$. Now, $\mathbf{e}_1 - \mathbf{e}_3$ is not periodic in P_7, while pair PST happens between $\mathbf{e}_1 - \mathbf{e}_7$ and $\mathbf{e}_3 - \mathbf{e}_5$ at time $\frac{\pi}{\sqrt{2}}$ by Example 5.5.4(1b). The same conclusion holds when $\mathbf{e}_v - \mathbf{e}_x = \mathbf{v}_-$.

Combining these cases yields the forward direction. The converse is immediate. □

An analogous argument yields P_3 as the only path admitting plus state transfer, between $\mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{e}_3 + \mathbf{e}_2$ in P_3 at time $\frac{\pi}{\sqrt{2}}$.

Corollary 9.7.2. *Plus state transfer occurs in P_n relative to A if and only if $n = 3$.*

Despite the rarity of vertex, pair and plus PST in P_n relative to A, Theorem 6.4.6 guarantees infinite families of paths that admit PST between real pure states.

Adapting the proof of Corollary 9.7.1, we get the following result relative to L.

Corollary 9.7.3. *Pair perfect state transfer occurs in P_n relative to L if and only if $n \in \{3, 4\}$. Plus perfect state transfer occurs in P_n relative to L if and only if $n = 4$.*

We close this section with the following observations.

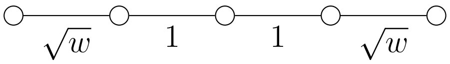

Figure 9.2: The weighted path $P_5(w)$

Example 9.7.4. We observe the following about P_n for $n \in \{3,4,5\}$ relative to L.

1. In P_3, $\mathbf{e}_1 - \mathbf{e}_2$ and $\mathbf{e}_3 - \mathbf{e}_2$ admit PST at $\frac{\pi}{2}$. Moreover, $\mathbf{e}_1 + \mathbf{e}_2$ and $\mathbf{e}_3 + \mathbf{e}_2$ are strongly cospectral and periodic with $\Phi^{+}_{\mathbf{x},\mathbf{y}}(L) = \{0,3\}$ and $\Phi^{-}_{\mathbf{x},\mathbf{y}}(L) = \{1\}$, but they do not admit PST as the conclusion of Corollary 6.1.9(3) does not hold.
2. In P_4, the pair $\{\mathbf{e}_1 + \mathbf{e}_4, \mathbf{e}_2 + \mathbf{e}_3\}$ admits PST at $\frac{\pi}{2}$, the pair $\{\mathbf{e}_1 - \mathbf{e}_2, \mathbf{e}_3 - \mathbf{e}_4\}$ admits PST at $\frac{\pi}{\sqrt{2}}$, and the pairs $\{\mathbf{e}_1 - \mathbf{e}_2, \mathbf{e}_3 - \mathbf{e}_4\}$, $\{\mathbf{e}_2 - \mathbf{e}_3, \frac{1}{\sqrt{2}}(\mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_3 - \mathbf{e}_4)\}$ and $\{\mathbf{e}_1 - \mathbf{e}_4, \frac{1}{\sqrt{2}}(\mathbf{e}_1 + \mathbf{e}_2 - \mathbf{e}_3 - \mathbf{e}_4)\}$ admit PST at $\frac{\pi}{2\sqrt{2}}$.
3. In P_5, the following pairs admit PST at $\frac{\pi}{\sqrt{5}}$: $\{\mathbf{e}_1 - \mathbf{e}_5, \frac{1}{\sqrt{5}}(\mathbf{e}_1 + 2\mathbf{e}_2 - 2\mathbf{e}_4 - \mathbf{e}_5)\}$ and $\{\mathbf{e}_2 - \mathbf{e}_4, \frac{1}{\sqrt{5}}(2\mathbf{e}_1 - \mathbf{e}_2 + \mathbf{e}_4 - 2\mathbf{e}_5)\}$.

In [28], edge PST relative to L was characterised for paths. It turns out that P_n admits pair PST relative to L if and only if it admits edge PST relative to L.

Lastly, we show that s-pair state transfer is possible for paths when $s \neq \pm 1$.

Example 9.7.5. For a positive real number w, consider the weighted path $P_5(w)$ in Figure 9.2. One checks that $P_5(w)$ has s-pair state transfer from $\mathbf{e}_3 - \frac{2}{\sqrt{w}}\mathbf{e}_1$ to $\mathbf{e}_3 - \frac{2}{\sqrt{w}}\mathbf{e}_5$ at time $\frac{\pi}{\sqrt{w}}$. Note that $s \neq \pm 1$ whenever $w \neq 4$. Moreover, the unweighted path P_5 has (-2)-pair state transfer between $\mathbf{e}_3 - 2\mathbf{e}_1$ to $\mathbf{e}_3 - 2\mathbf{e}_5$ at time π.

9.8 Distance-regular graphs

A *distance-regular graph* (DRG) is a regular graph such that for any two vertices v and w, the number of vertices at distance j from v and at distance k from w depends only upon j, k, and the distance between v and w. A connected distance-regular graph of diameter one is a complete graph, while a connected distance-regular graph of diameter two is called a *strongly-regular graph.* A distance-regular graph is *antipodal* if its diameter is d and the relation on vertices "is equal to or at distance d from" is an equivalence relation. The equivalence classes are called *fibres.* If a distance-regular graph is antipodal, then the fibres all have same size. A cycle on an even number of vertices is an example of an antipodal distance-regular graph with fibres of size two. A cycle on an odd number of vertices is also a distance-regular graph albeit non-antipodal. Strongly regular graphs, which includes the family of conference graphs, are distance-regular graphs of diameter two. The hypercubes Q_d are also antipodal distance-regular with fibres of size two and diameter d. See [17] for a background of distance-regular graphs.

In this section, we determine all occurrences of s-pair state transfer in cycles and antipodal distance-regular graphs (DRGs) that have vertex PST whenever $s \in \mathbb{R}\backslash\{0\}$. We start with cycles.

9.8.1 Cycles

Let $n \geq 4$. For $j \in \{0, \ldots, \lfloor \frac{n}{2} \rfloor\}$, consider the eigenvalue $\theta_j = 2\cos(2j\pi/n)$ of $A(C_n)$. Making use of the eigenvectors of $A(C_n)$ in Lemma 5.4.1, we obtain the spectral idempotent E_j associated with λ_j. The (a,b)-entry of E_j is given

$$\begin{cases} \dfrac{1}{n} & \text{if } j = 0, \\ \dfrac{2}{n}\cos\left(\dfrac{2\pi j(a-b)}{n}\right) & \text{if } 1 \leq j < \frac{n}{2}, \\ \dfrac{(-1)^{a+b}}{n} & \text{if } n \text{ is even and } j = \frac{n}{2}, \end{cases} \tag{9.8.1}$$

for $a, b \in \mathbb{Z}_n$ and for $j = 0, \ldots, \lfloor \frac{n}{2} \rfloor$.

To determine s-pair state transfer in C_n, it suffices to determine which s-pair states admit PST with $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_b$, for some $b \in \{1, 2, \ldots, \lfloor \frac{n}{2} \rfloor\}$ and $s \in \mathbb{R}\backslash\{0\}$. Note that $\lambda_j \in \Phi_{\mathbf{u}}$ if and only if $E_j(\mathbf{e}_0 + s\mathbf{e}_b) \neq \mathbf{0}$.

By Corollary 6.1.8, periodicity is a necessary condition for real state transfer. So our approach is to first classify periodic s-pair states $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_b$ in C_n, for $s = 1$, $s = -1$ and $s \neq \pm 1$. The following result [69] is useful in our proofs.

Lemma 9.8.1. *If* $\cos \frac{2\pi}{n} \in \mathbb{Q}$, *then* $n \in \{1, 2, 3, 4, 6\}$. *If the minimal polynomial of* $\cos \frac{2\pi}{n}$ *has degree two, then* $n \in \{5, 8, 10, 12\}$.

We now characterise pair state periodicity in C_n.

Lemma 9.8.2. *Let* $n \geq 4$. *The plus state* $\mathbf{u} = \mathbf{e}_0 + \mathbf{e}_b$, *for* $1 \leq b \leq \frac{n}{2}$, *is periodic in* C_n *with minimum period* ρ *if and only if the triple* $(n, \mathbf{e}_b, \rho)$ *belongs to*

$$\left\{(4, \mathbf{e}_1, \pi), \left(4, \mathbf{e}_2, \frac{\pi}{2}\right), (6, \mathbf{e}_1, 2\pi), (6, \mathbf{e}_2, 2\pi), \left(6, \mathbf{e}_3, \frac{2\pi}{3}\right), (8, \mathbf{e}_4, \pi), (12, \mathbf{e}_6, 2\pi)\right\}.$$

Proof. Suppose $\mathbf{u}$ is periodic. From (9.8.1), for $1 \leq j < \frac{n}{2}$,

$$\mathbf{e}_0^T E_{\lambda_j} \mathbf{u} = \frac{2}{n}\left(\cos\frac{2\pi bj}{n} + 1\right).$$

Hence $\lambda_j \in \Phi_{\mathbf{u}}$ when $\frac{bj}{n} - \frac{1}{2} \notin \mathbb{Z}$. If $b \neq \frac{n}{2}$ then $\lambda_0, \lambda_1 \in \Phi_{\mathbf{u}}$. Since $\lambda_0 = 2$, Lemma 3.3.7 and Theorem 3.7.10 imply $2\cos\frac{2\pi}{n} \in \mathbb{Z}$. Similarly, if $b = \frac{n}{2}$ then $\lambda_0, \lambda_2 \in \Phi_{\mathbf{u}}$ and $2\cos\frac{4\pi}{n} \in \mathbb{Z}$. It follows from Lemma 9.8.1 that $n \in \{4, 6, 8, 12\}$. One may then check all plus states $\mathbf{e}_0 + \mathbf{e}_b$ that satisfy the conditions in Theorem 3.7.10 to get the list above. The minimum period of each case is computed using the expression given in Theorem 3.7.10. ☐

For plus state periodicity, we have the following result.

Lemma 9.8.3. *Let $n \geq 4$. The pair state $\mathbf{u} = \mathbf{e}_0 - \mathbf{e}_b$, for $1 \leq b \leq \frac{n}{2}$, is periodic in C_n if and only if*

$$\begin{aligned}(n, \mathbf{e}_b, \rho) \quad \in \quad & \Bigg\{ (4, \mathbf{e}_1, \pi), \left(5, \mathbf{e}_1, \frac{2\pi}{\sqrt{5}}\right), \left(5, \mathbf{e}_2, \frac{2\pi}{\sqrt{5}}\right), (6, \mathbf{e}_1, 2\pi), (6, \mathbf{e}_2, \pi), \\ & \left(6, \mathbf{e}_3, \frac{2\pi}{3}\right), \left(8, \mathbf{e}_2, \frac{2\pi}{\sqrt{2}}\right), \left(8, \mathbf{e}_4, \frac{\pi}{\sqrt{2}}\right), \left(12, \mathbf{e}_6, \frac{2\pi}{\sqrt{3}}\right) \Bigg\}.\end{aligned}$$

Moreover, $(\mathbf{e}_0 - \mathbf{e}_2)$ is a fixed state of C_4.

Proof. Suppose $\mathbf{u}$ is periodic. From (9.8.1), for $1 \leq j < \frac{n}{2}$,

$$\mathbf{e}_0^T E_{\lambda_j} \mathbf{u} = \frac{2}{n}\left(\cos\frac{2\pi bj}{n} - 1\right).$$

Hence $\lambda_j \in \Phi_{\mathbf{u}}$ if $\frac{bj}{n} \notin \mathbb{Z}$. If $1 \leq b < \frac{n}{2}$ then $\lambda_1, \lambda_2 \in \Phi_{\mathbf{u}}$. If follows from Corollary 3.7.18 that $|\lambda_2 - \lambda_1| \geq 1$ which implies $n \leq 10$. Similarly, if $b = \frac{n}{2}$ then $\lambda_j \in \Phi_{\mathbf{u}}$ for odd j. Lemma 3.3.7 and Theorem 3.7.10 and Lemma 9.8.1 then imply that $n \in \{4, 5, 6, 8, 10, 12\}$. The same argument as the previous lemma yields the desired conclusion. ☐

Lemma 9.8.4. *For $s \in \mathbb{C}\backslash\{\pm 1\}$, the s-pair state $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_b$ is periodic in C_n with period ρ if and only if one of the following holds.*

1. *$n = 4$, $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_b$ is periodic with $\rho = \pi$, for $1 \leq b \leq 3$ and $s \in \mathbb{R}\backslash\{\pm 1\}$.*

2. *$n = 6$, $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_b$ is periodic with $\rho = 2\pi$, for $1 \leq b \leq 5$ and $s \in \mathbb{R}\backslash\{\pm 1\}$.*

Proof. It follows from Proposition 9.4.6 that 0 and b are periodic vertices in C_n, and C_4 and C_6 are the only cycles with periodic vertices. Now, 1 follows from the fact that the transition matrix for C_4 is equal to the identity matrix at minimum time π. Meanwhile, 2 follows from the fact that the transition matrix for C_6 is equal to the identity matrix at minimum time 2π. □

Theorem 9.8.5. *Let $s \in \mathbb{R}\backslash\{0\}$. In C_n, s-pair state transfer occurs from $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_b$ to $\boldsymbol{\mu} = \mathbf{e}_u + s\mathbf{e}_v$ at time τ for $1 \leq b \leq \frac{n}{2}$ relative to $\alpha D + A$ if and only if one of the following conditions holds.*

1. $n = 4$, $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_1$, $\boldsymbol{\mu} = \mathbf{e}_2 + s\mathbf{e}_3$, $\tau = \frac{\pi}{2}$, *for any* $s \in \mathbb{R}\backslash\{0\}$.
2. $n = 4$, $\mathbf{u} = \mathbf{e}_0 + s\mathbf{e}_2$, $\boldsymbol{\mu} = \mathbf{e}_2 + s\mathbf{e}_0$, $\tau = \frac{\pi}{2}$, *for any* $s \in \mathbb{R}\backslash\{0, \pm 1\}$.
3. $n = 4$, $\mathbf{u} = \mathbf{e}_0 + \mathbf{e}_2$, $\boldsymbol{\mu} = \mathbf{e}_1 + \mathbf{e}_3$, $\tau = \frac{\pi}{4}$.
4. $n = 6$, $\mathbf{u} = \mathbf{e}_0 - \mathbf{e}_2$, $\boldsymbol{\mu} = \mathbf{e}_3 - \mathbf{e}_5$, $\tau = \frac{\pi}{2}$.
5. $n = 6$, $\mathbf{u} = \mathbf{e}_0 + 2\mathbf{e}_2$, $\boldsymbol{\mu} = \mathbf{e}_0 + 2\mathbf{e}_4$, $\tau = \pi$.
6. $n = 6$, $\mathbf{u} = \mathbf{e}_0 + \frac{1}{2}\mathbf{e}_2$, $\boldsymbol{\mu} = \mathbf{e}_4 + \frac{1}{2}\mathbf{e}_2$, $\tau = \pi$.
7. $n = 8$, $\mathbf{u} = \mathbf{e}_0 - \mathbf{e}_2$, $\boldsymbol{\mu} = \mathbf{e}_4 - \mathbf{e}_6$, $\tau = \frac{\pi}{\sqrt{2}}$.
8. $n = 8$, $\mathbf{u} = \mathbf{e}_0 + \mathbf{e}_4$, $\boldsymbol{\mu} = \mathbf{e}_2 + \mathbf{e}_6$, $\tau = \frac{\pi}{2}$.

Proof. By Corollary 6.1.1(2), it suffices to check if perfect s-pair state transfer occurs at half of the minimum periods list in Lemmas 9.8.2, 9.8.3 and 9.8.4. □

From Theorem 9.8.5, we have the following result.

Corollary 9.8.6. *If $n \geq 9$, then C_n does not admit perfect state transfer between real s-pair states relative to $\alpha D + A$.*

Example 9.8.7. In C_8, the pairs $\{\mathbf{e}_0 - \mathbf{e}_2, \mathbf{e}_4 - \mathbf{e}_6\}$ and $\{\mathbf{e}_0 + \mathbf{e}_4, \mathbf{e}_2 + \mathbf{e}_6\}$ admit PST by Theorem 9.8.5(7-8). Moreover, $\mathbf{e}_0 + \mathbf{e}_2 + \mathbf{e}_4 + \mathbf{e}_6$ and $\mathbf{e}_1 + \mathbf{e}_3 + \mathbf{e}_5 + \mathbf{e}_7$ admit PST in C_8 by Example 6.1.7. This is illustrated in Figure 9.3, where vertices with the same colour (blue or pink) indicate a single pure state.

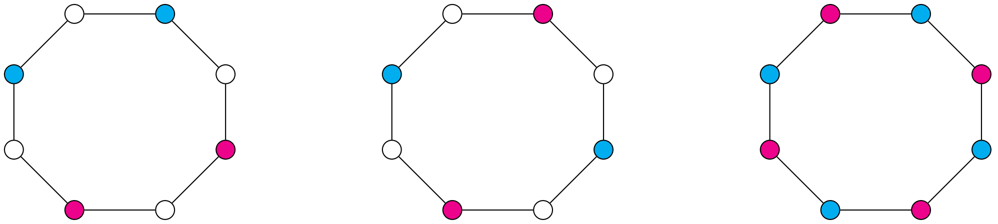

Figure 9.3: Real state transfer in C_8: $\mathbf{e}_0 - \mathbf{e}_2$ and $\mathbf{e}_4 - \mathbf{e}_6$ (left), between $\mathbf{e}_0 + \mathbf{e}_4$ and $\mathbf{e}_2 + \mathbf{e}_6$ (center), and between $\mathbf{e}_0 + \mathbf{e}_2 + \mathbf{e}_4 + \mathbf{e}_6$ and $\mathbf{e}_1 + \mathbf{e}_3 + \mathbf{e}_5 + \mathbf{e}_7$ (right)

9.8.2 Antipodal DRGs

In [38], it was proved that if a distance-regular graph X admits vertex PST and d is the diameter of X, then X is an antipodal distance-regular graph with fibres of size two. That is, there is a unique vertex in X that is at distance d from a given vertex. In this case, perfect state transfer occurs between the vertex states determined by those two vertices in each fibre. Please see [38] for a list of distance-regular graphs that have vertex PST, which includes the hypercubes Q_d for all $d \geq 1$.

Suppose X is an antipodal distance-regular graph with fibres of size two and diameter d. For $j \in \{0, 1, \ldots, d\}$, let A_j be the j-th distance matrix of X. That is, the (u, v) entry of A_j is equal to 1 if u and v are at distance j, and 0 otherwise. Note that $A_0 = I$, A_d is the anti-diagonal permutation matrix (up to permutation of vertices), and

$$A_j A_d = A_{d-j}, \quad \text{for } j = 0, \ldots, d.$$

Let k_j be the column sum of A_j, for $j = 0, \ldots, d$. Then $k_0 = k_d = 1$ and the sequence $k_0, k_1, \ldots, k_{d-1}, k_d$ is unimodal, see Theorem 5.1.1 (i) of [17]. Further, if X is not a cycle then Theorem 5.1.1 (ii) of [17] implies that $k_j \geq 3$, for $j = 1, \ldots, d-1$.

Let $\mathcal{A}$ be the matrix algebra over $\mathbb{C}$ generated by the set $\{A_0, A_1, \ldots, A_d\}$. From (3.1.2), we obtain

$$U_A(t) \in \text{span } \{A_0, A_1, \ldots, A_d\}.$$

If X admits perfect state transfer between two vertices at time τ then

$$U_A(\tau) = \eta A_d, \tag{9.8.2}$$

for some phase factor η.

Theorem 9.8.8. *Let $s \in \mathbb{C}\backslash\{0\}$ and X be a distance-regular graph that is not a cycle. If X admits perfect state transfer between vertices relative to $\alpha D + A$, then*

X has s-pair state transfer from $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ to $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ whenever one of the following holds.

1. *$\{a, b\}$ is not an antipodal pair, $\{a, \alpha\}$ and $\{b, \beta\}$ are antipodal pairs.*
2. *$\{a, b\}$ is an antipodal pair, $\alpha = b$ and $\beta = a$, for $s \in \mathbb{C}\backslash\{0, \pm 1\}$.*

Moreover, if we restrict $s \in \mathbb{R}\backslash\{0\}$, then X has s-pair state transfer from $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ to $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_\beta$ if and only if one of the two conditions above holds.

Proof. Let d be the diameter of X, and let τ be the minimum PST time between $\mathbf{e}_u$ and $\mathbf{e}_v$ in X, where u and v are antipodal vertices in X.

First, suppose $\text{dist}(a, b) < d$. Let α and β be vertices in X that are antipodal to a and b, respectively. From (9.8.2), we obtain $U(\tau)\mathbf{u} = \eta\boldsymbol{\mu}$. Next, suppose $\text{dist}(a, b) = d$, that is, $\mathbf{e}_b = A_d\mathbf{e}_a$. Then (9.8.2) again yields $U(\tau)\mathbf{u} = \eta\boldsymbol{\mu}$. Thus, the desired conclusion holds for conditions 1 and 2.

If we restrict $s \in \mathbb{R}$, then both $\mathbf{u}$ and $\boldsymbol{\mu}$ in condition 1 are real states, and so it follows from Corollary 4.4.5 that PST does not occur from $\mathbf{u}$ to another real state. Meanwhile, in condition 2, $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ and $\boldsymbol{\mu} = \mathbf{e}_b + s\mathbf{e}_a$ represent distinct real states whenever $s \neq \pm 1$ and so Corollary 4.4.5 once again implies PST does not occur from $\mathbf{u}$ to another s-pair state. To complete the proof, we show that $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_b$ does not admit PST whenever $s \in \{\pm 1\}$ and $\{a, b\}$ is an antipodal pair. By virtue of (9.8.2), we have $U(\tau)(\mathbf{e}_a + s\mathbf{e}_b) = s\eta(\mathbf{e}_b + s\mathbf{e}_a)$, and so in this case, $\mathbf{u}$ is periodic at time τ. Moreover, since $\{a, b\}$ is an antipodal pair, we have $\mathbf{u} = (I + sA_d)\mathbf{e}_a$. Now, let τ' be the minimum period of $\mathbf{u}$, and suppose

$$U\left(\frac{\tau'}{2}\right) = \sum_{j=0}^{d} \varphi_j A_j,$$

for some $\varphi_0, \ldots, \varphi_d \in \mathbb{C}$. Then

$$U\left(\frac{\tau'}{2}\right)\mathbf{u} = U\left(\frac{\tau'}{2}\right)(I + sA_d)\mathbf{e}_a = \sum_{j=0}^{d} (\varphi_j + s\varphi_{d-j})\, A_j\mathbf{e}_a.$$

Using the fact that $A_0 = I$ and A_d is the anti-diagonal permutation matrix, if there exists $1 \leq j \leq d-1$ such that $\varphi_j + s\varphi_{d-j} \neq 0$, then $U\left(\frac{\tau'}{2}\right)(\mathbf{e}_a + s\mathbf{e}_b)$ has at least $k_j \geq 3$

non-zero entries because X is not a cycle, so it is not an s-pair state. Otherwise,

$$\begin{aligned} U\left(\frac{\tau'}{2}\right)\mathbf{u} &= U\left(\frac{\tau'}{2}\right)(I+sA_d)\mathbf{e}_a \\ &= \left((\varphi_0+s\varphi_d)I+(\varphi_d+s\varphi_0)A_d\right)\mathbf{e}_a \\ &= (\varphi_0+s\varphi_d)\left(I+sA_d\right)\mathbf{e}_a \\ &= (\varphi_0+s\varphi_d)\mathbf{u}, \end{aligned}$$

which contradicts the assumption that τ' is the minimum period of $\mathbf{u}$. This proves that $\mathbf{e}_a \pm \mathbf{e}_b$ does not admit s-pair state transfer in X. □

The cycle C_4 is the only cycle admitting vertex PST. From Theorem 9.8.5, C_6 and C_8 are the only other cycles that have s-pair state transfer.

Remark 9.8.9. In Theorem 9.8.8, if $\{a, b\}$ is not an antipodal pair, $\{a, \alpha\}$ and $\{b, \beta\}$ are antipodal pairs, then

$$U(\tau)(\mathbf{e}_a+s\mathbf{e}_b)=\eta(\mathbf{e}_\alpha+s\mathbf{e}_\beta)=s\eta(\mathbf{e}_\beta+\overline{s}\mathbf{e}_\alpha) \tag{9.8.3}$$

whenever s is a unit complex number. Similarly, if $\{a, b\}$ is an antipodal pair, then

$$U(\tau)(\mathbf{e}_a+s\mathbf{e}_b)=\eta(\mathbf{e}_b+s\mathbf{e}_a)=s\eta(\mathbf{e}_a+\overline{s}\mathbf{e}_b). \tag{9.8.4}$$

This gives us an infinite family of graphs that admit PST between an s-pair state and an $\overline{s}$-pair state. This also complements Remark 9.0.3.

9.9 Constructions

In this section, we construct more infinite families of graphs admitting s-pair state transfer. We start with a result that is immediate from Theorem 4.7.2.

Theorem 9.9.1. *Let $s \in \mathbb{C}\backslash\{0\}$. If the pairs $\{\mathbf{e}_a, \mathbf{e}_\alpha\}$ and $\{\mathbf{e}_b, \mathbf{e}_\beta\}$ admit perfect state transfer at the same time τ and the same phase factor γ, then $\mathbf{u}=\mathbf{e}_a+s\mathbf{e}_b$ and $\boldsymbol{\mu}=\mathbf{e}_\alpha+s\mathbf{e}_\beta$ also admit perfect state transfer at time τ and phase factor γ.*

Next, we characterise perfect state transfer between s-pair states of the form $\mathbf{u}=\mathbf{e}_a+s\mathbf{e}_b$ and $\boldsymbol{\mu}=\mathbf{e}_b+s\mathbf{e}_a$.

Theorem 9.9.2. *Let $s \in \mathbb{C}\backslash\{0\}$, $\mathbf{u}=\mathbf{e}_a+s\mathbf{e}_b$ and $\boldsymbol{\mu}=\mathbf{e}_b+s\mathbf{e}_a$.*

1. *Let $s=\pm 1$. If perfect state transfer occurs between $\mathbf{e}_a$ and $\mathbf{e}_b$, then $\mathbf{u}$ is periodic.*

2. *Let $s \neq \pm 1$. Then perfect state transfer occurs between $\mathbf{e}_a$ and $\mathbf{e}_b$ if and only if s-pair state transfer occurs from $\mathbf{u}$ to $\boldsymbol{\mu}$ at the same time.*

Proof. First, suppose $U(\tau)\mathbf{e}_a = \gamma\mathbf{e}_b$. Since $\mathbf{e}_a$ and $\mathbf{e}_b$ are real states, PST in this case is symmetric by Corollary 6.1.3, and so $U(\tau)\mathbf{e}_b = \gamma\mathbf{e}_a$. Consequently

$$U(\tau)(\mathbf{e}_a + s\mathbf{e}_b) = \gamma(\mathbf{e}_b + s\mathbf{e}_a).$$

From the above equation, 1 and the forward implication in 2 are straightforward. We now prove the converse of 2. Suppose s-pair state transfer occurs from $\mathbf{u}$ to $\boldsymbol{\mu}$, where $s \neq \pm 1$. Then $\mathbf{u}$ and $\boldsymbol{\mu}$ are strongly cospectral. That is, $E_\lambda \mathbf{u} = \zeta_\lambda E_\lambda \boldsymbol{\mu}$ for all $\lambda \in \Phi_{\mathbf{u}}$, where z_λ is a unit complex number. Equivalently,

$$(1 - z_\lambda s)E_\lambda \mathbf{e}_a = (z_\lambda - s)E_\lambda \mathbf{e}_b.$$

In this case, $\mathbf{e}_a$ and $\mathbf{e}_b$ are strongly cospectral if and only if $\frac{z_\lambda - s}{1 - z_\lambda s}$ is a unit complex number, or equivalently, $|z_\lambda - s| = |1 - z_\lambda s|$. Since $|z_\lambda| = 1$, this implies that $z_\lambda \in \mathbb{R}$ or $s \in \mathbb{R}$. If $z_\lambda \in \mathbb{R}$, then $z_\lambda = \pm 1$, and the above equation implies that $\mathbf{e}_a$ and $\mathbf{e}_b$ are strongly cospectral. On the other hand, if $s \in \mathbb{R}$, then $\mathbf{u}$ and $\boldsymbol{\mu}$ are real states, and so each ζ_λ must be equal to ± 1. Since $s \neq \pm 1$, we get that $E_\lambda \mathbf{u} = E_\lambda \boldsymbol{\mu}$ if and only if $E_\lambda \mathbf{e}_a = E_\lambda \mathbf{e}_b$, while $E_\lambda \mathbf{u} = -E_\lambda \boldsymbol{\mu}$ if and only if $E_\lambda \mathbf{e}_a = -E_\lambda \mathbf{e}_b$. In both cases, we get that $\mathbf{e}_a$ and $\mathbf{e}_b$ are strongly cospectral with

$$\Phi^+_{\mathbf{e}_a,\mathbf{e}_b} = \Phi^+_{\mathbf{u},\boldsymbol{\mu}} \quad \text{and} \quad \Phi^-_{\mathbf{e}_a,\mathbf{e}_b} = \Phi^-_{\mathbf{u},\boldsymbol{\mu}}.$$

These equalities imply that $\mathbf{u}$ and $\boldsymbol{\mu}$ satisfy conditions 1 or 2 in Corollary 6.1.8 if and only if $\mathbf{e}_a$ and $\mathbf{e}_b$ satisfy them as well. Thus, PST occurs between $\mathbf{e}_a$ and $\mathbf{e}_b$. ☐

Remark 9.9.3. The converse of Theorem 9.9.2(1) does not hold in general. For instance, if $s = -1$ and $M = A$, then we may take a conference graph X and the pair state $\mathbf{u} = \mathbf{e}_a - \mathbf{e}_b$. From Example 9.4.7, $\mathbf{u}$ is periodic in X, but $\mathbf{e}_a$ and $\mathbf{e}_b$ are not involved in PST in X because they are not periodic. Now, for $s = 1$ and $M = A$, we may consider P_4 with end vertices a, b. Then $|\Phi_{\mathbf{u}}| = 2$, and so $\mathbf{u}$ is periodic Theorem 3.7.3. However, $\Phi_{\mathbf{e}_a} = \Phi_{\mathbf{e}_b} = \{\pm(1 \pm \sqrt{5})/2\}$ does not satisfy the ratio condition, and so $\mathbf{e}_a$ and $\mathbf{e}_b$ are not involved in PST by Corollary 6.1.1(2).

However, there are times when the converse of Theorem 9.9.2(1) holds. For instance, if $s = 1$ and $M = A$, we may consider P_3 with end vertices a, b which is known to admit PST at $\frac{\pi}{\sqrt{2}}$. Since $|\Phi_{\mathbf{u}}| = 2$, $\mathbf{u}$ is also periodic by Theorem 3.7.3.

Theorem 9.9.4. *Let $s \in \mathbb{C}\backslash\{0\}$. Suppose perfect state transfer occurs between $\mathbf{e}_a$ and $\mathbf{e}_\alpha$ at time τ and $\mathbf{e}_v$ is periodic at τ. Then s-pair state transfer occurs from $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_v$ to $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_v$ at time τ if and only if there exist $\lambda \in \Phi^+_{\mathbf{e}_a,\mathbf{e}_\alpha} \cap \Phi_{\mathbf{u}}$ and $\lambda' \in \Phi_{\mathbf{e}_v} \cap \Phi_{\mathbf{u}}$ such that*

$$\tau(\lambda - \lambda') \equiv 0 \pmod{2\pi}.$$

Proof. Let $\lambda \in \Phi^+_{\mathbf{e}_a,\mathbf{e}_\alpha}$ and $\lambda' \in \Phi_{\mathbf{e}_v}$. By Theorem 4.1.3 and (3.7.2), the phase factors for PST and periodicity are $e^{\mathrm{i}\tau\lambda}$ and $e^{\mathrm{i}\tau\lambda'}$. Consequently,

$$U(\tau)\mathbf{e}_a = e^{-\mathrm{i}\tau\lambda}\mathbf{e}_\alpha \quad \text{and} \quad U(\tau)\mathbf{e}_v = e^{-\mathrm{i}\tau\lambda'}\mathbf{e}_v.$$

From this, it follows that

$$U(\tau)\left(\mathbf{e}_a + s\mathbf{e}_v\right) = e^{\mathrm{i}\tau\lambda}\mathbf{e}_\alpha + se^{\mathrm{i}\tau\lambda'}\mathbf{e}_v = \eta\left(\mathbf{e}_\alpha + s\mathbf{e}_v\right)$$

if and only if $\lambda \in \Phi^+_{\mathbf{e}_a,\mathbf{e}_\alpha} \cap \Phi_{\mathbf{u}}$, $\lambda' \in \Phi_{\mathbf{e}_v} \cap \Phi_{\mathbf{u}}$ and $e^{\mathrm{i}\tau\lambda} = e^{\mathrm{i}\tau\lambda'} = \eta$. The latter condition is equivalent to $\tau(\lambda - \lambda') \equiv 0 \pmod{2\pi}$. □

Remark 9.9.5. If M is a nonnegative matrix, say $M \in \{A, Q\}$ and $\mathbf{u}^T\mathbf{v} \neq 0$ where $\mathbf{v}$ is a Perron eigenvector for M, then the condition on the eigenvalue supports in Theorem 9.9.4 holds whenever we take $\lambda = \lambda'$ to be the Perron eigenvalue of M. Moreover, if $M = L$ and $s \neq -1$, then Theorem 9.9.4 also applies with $\lambda = \lambda' = 0$.

Example 9.9.6. Consider P_3 with $V(P_3) = \{1, 2, 3\}$, where vertex 2 has degree two. At $\tau = \frac{\pi}{\sqrt{2}}$, the transition matrix relative to A is given by

$$U_A(\tau) = -\begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}. \tag{9.9.1}$$

For any positive integer d, (3.6.4) implies that the transition matrix of the Cartesian power $P_3^{\square d}$ is $U_A(t)^{\otimes d}$. From (9.9.1), $U_A(\tau)^{\otimes d}$ is an antidiagonal permutation matrix up to a scalar factor of $(-1)^d$. Thus, $P_3^{\square d}$ has perfect state transfer from vertex $a = (1, 1, \ldots, 1)$ to vertex $\alpha = (3, 3, \ldots, 3)$ at time τ, and is periodic at the vertex $v = (2, 2, \ldots, 2)$ at the same time. Note that $d\sqrt{2} \in \Phi^+_{\mathbf{e}_a,\mathbf{e}_\alpha} \cap \Phi_{\mathbf{e}_v}$ is the Perron eigenvalue for $P_3^{\square d}$ with associated Perron eigenvector

$$\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}^{\otimes d}.$$

Now, let $\mathbf{u} = \mathbf{e}_a + s\mathbf{e}_v$ and $\boldsymbol{\mu} = \mathbf{e}_\alpha + s\mathbf{e}_v$. Then we have $d\sqrt{2} \in \Phi_{\mathbf{u}}$ if and only if

$$\left(\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}^{\otimes d}\right)^T \mathbf{u} = \left(\begin{bmatrix} 1 \\ \sqrt{2} \\ 1 \end{bmatrix}^{\otimes d}\right)^T (\mathbf{e}_1^{\otimes d} + s\mathbf{e}_2^{\otimes d}) = 1 + s(\sqrt{2})^d \neq 0.$$

Equivalently, $s \neq -\frac{1}{\sqrt{2}^d}$. Invoking Theorem 9.9.4, we get PST from $\mathbf{u}$ to $\boldsymbol{\mu}$ in $P_3^{\square d}$ relative to A at time τ for all $s \in \mathbb{C} \backslash \left\{0, -\frac{1}{\sqrt{2}^d}\right\}$.

Next, we utilise Cartesian products to get more examples of s-pair state transfer. The following is immediate from Theorem 4.7.3.

Corollary 9.9.7. *Let $(r, s) \in \mathbb{C}^2 \backslash \{(0, 0)\}$ and suppose perfect state transfer from $\mathbf{e}_a + s\mathbf{e}_b$ to $\mathbf{e}_c + r\mathbf{e}_d$ at time τ relative to M_2, where $\{a, b\} \neq \{c, d\}$ whenever $r = s$.*

1. *If perfect state transfer occurs between vertex states $\mathbf{e}_u$ and $\mathbf{e}_v$ at time τ relative to M_1, then perfect state transfer occurs from $\mathbf{e}_u \otimes (\mathbf{e}_a + s\mathbf{e}_b)$ to $\mathbf{e}_v \otimes (\mathbf{e}_c + r\mathbf{e}_d)$ at time τ relative to $M_1 \otimes I + I \otimes M_2$.*
2. *If $\mathbf{e}_u$ is periodic at time τ relative to M_1, then perfect state transfer from $\mathbf{e}_u \otimes (\mathbf{e}_a + s\mathbf{e}_b)$ to $\mathbf{e}_u \otimes (\mathbf{e}_c + r\mathbf{e}_d)$ at time τ relative to $M_1 \otimes I + I \otimes M_2$.*

If M_1 and M_2 are taken to be $\alpha D + A$, then the above result applies to the Cartesian product $X \square Y$, where $M_1 = \alpha D(X) + A(X)$ and $M_2 = \alpha D(Y) + A(Y)$. Moreover, since $\mathbf{e}_u \otimes (\mathbf{e}_a + s\mathbf{e}_b)$ is an s-pair state in $X \square Y$, the above corollary can be used to construct infinite families of graphs with s-pair PST.

Example 9.9.8. From Example 3.6.1, we know that the hypercube Q_d of dimension $d \geq 1$ admits PST between $\mathbf{e}_u$ and $\mathbf{e}_v$ at time $\frac{\pi}{2}$, where u and v are any pair of antipodal vertices. The following hold for all $d \geq 1$.

- By Corollary 9.9.7(1) and Example 5.4.5(1a), the pairs $\{\mathbf{e}_u \otimes (\mathbf{e}_0 + \mathbf{e}_4), \mathbf{e}_v \otimes (\mathbf{e}_2 + \mathbf{e}_6)\}$ and $\{\mathbf{e}_u \otimes (\mathbf{e}_0 + \mathbf{e}_4 + \mathbf{e}_8), \mathbf{e}_v \otimes (\mathbf{e}_2 + \mathbf{e}_6 + \mathbf{e}_{10})\}$ admit PST in $Q_d \square C_8$ and $Q_d \square C_{12}$ relative to $\alpha D + A$ at $\frac{\pi}{2}$, respectively.
- By Corollary 9.9.7 and Theorem 9.8.5(4-6), $Q_d \square C_6$ admits PST between the pair $\{\mathbf{e}_u \otimes (\mathbf{e}_0 - \mathbf{e}_2), \mathbf{e}_v \otimes (\mathbf{e}_3 - \mathbf{e}_5)\}$ at $\frac{\pi}{2}$, and between the pairs $\{\mathbf{e}_u \otimes (\mathbf{e}_0 + 2\mathbf{e}_2), \mathbf{e}_u \otimes (\mathbf{e}_0 + 2\mathbf{e}_4)\}$ and $\{\mathbf{e}_u \otimes (\mathbf{e}_0 + \frac{1}{2}\mathbf{e}_2), \mathbf{e}_u \otimes (\mathbf{e}_4 + \frac{1}{2}\mathbf{e}_2)\}$ at π relative to $\alpha D + A$.
- By Corollary 9.9.7(1) and Example 9.7.4(1,2), we get PST in $Q_d \square P_3$ and $Q_d \square P_4$ relative to L between the pairs $\{\mathbf{e}_u \otimes (\mathbf{e}_1 - \mathbf{e}_2), \mathbf{e}_v \otimes (\mathbf{e}_3 - \mathbf{e}_2)\}$ and $\{\mathbf{e}_u \otimes (\mathbf{e}_1 + \mathbf{e}_4), \mathbf{e}_v \otimes (\mathbf{e}_2 + \mathbf{e}_3)\}$ at $\frac{\pi}{2}$, respectively.

Example 9.9.9. Let $M = A$ and consider $P_3^{\square n}$. By Example 9.9.6, $P_3^{\square n}$ admits PST at time $\frac{\pi}{\sqrt{2}}$ between $\mathbf{e}_u$ and $\mathbf{e}_v$, where $\{u, v\}$ is a pair of vertices at distance $2n$.

- By Corollary 9.9.7(1) and Example 5.5.4(1b), $(P_3^{\square n})\square P_7$ admits PST between $\mathbf{e}_u \otimes (\mathbf{e}_1 - \mathbf{e}_7)$ and $\mathbf{e}_v \otimes (\mathbf{e}_3 - \mathbf{e}_5)$ at $\frac{\pi}{\sqrt{2}}$ for all $n \geq 1$.
- By Corollary 9.9.7(1) and Theorem 9.8.5(7), $(P_3^{\square n})\square C_8$ admits PST between $\mathbf{e}_u \otimes (\mathbf{e}_0 - \mathbf{e}_2)$ and $\mathbf{e}_v \otimes (\mathbf{e}_4 - \mathbf{e}_6)$ at time $\frac{\pi}{\sqrt{2}}$ for all $n \geq 1$.

In Theorem 9.6.1(2b), we provided an infinite family that admits PST from an s-pair state to an $\overline{s}$-pair state where s is nonreal. The following example yields another infinite family with such a property.

Example 9.9.10. In Corollary 9.5.1(2), K_3 admits PST from $\mathbf{e}_1 + s\mathbf{e}_2$ to $\mathbf{e}_3 + (s-1)\mathbf{e}_2$ at time $\tau = \frac{\pi}{2}$, where $s = \frac{1}{2}(1 + 3\mathrm{i})$. Invoking Corollary 9.9.7(1), $Q_d \square K_3$ admits PST from $\mathbf{e}_u \otimes (\mathbf{e}_1 + s\mathbf{e}_2)$ to $\mathbf{e}_v \otimes (\mathbf{e}_3 - (s-1)\mathbf{e}_2)$ at time $\frac{\pi}{2}$ for all $d \geq 1$ relative to $\alpha D + A$, where u and v are antipodal vertices in Q_d. In this case, $-(s-1) = \overline{s}$.

Example 9.9.11. Let X be distance-regular graph that is not a cycle admitting vertex PST at time τ, and Y be a graph that has PST between $\mathbf{e}_u$ and $\mathbf{e}_v$ at τ. The following hold for all $s \in \mathbb{C}\backslash\{0\}$ relative to $\alpha D + A$.

- Suppose $\{a, b\}$ is not an antipodal pair and that $\{a, \alpha\}$ and $\{b, \beta\}$ are antipodal pairs. By Theorem 9.8.8(1) and Corollary 9.9.7, we get PST from $\mathbf{e}_u \otimes (\mathbf{e}_a + s\mathbf{e}_b)$ to $\mathbf{e}_v \otimes (\mathbf{e}_\alpha + s\mathbf{e}_\beta)$ at time τ. Additionally, if $|s| = 1$, then (9.8.3) yields PST from $\mathbf{e}_a \otimes (\mathbf{e}_u + s\mathbf{e}_b)$ to $\mathbf{e}_v \otimes (\mathbf{e}_\beta + \overline{s}\mathbf{e}_\alpha)$ at time τ.
- Let $s \notin \{0, \pm 1\}$ an suppose $\{a, b\}$ is an antipodal pair, $\alpha = b$ and $\beta = a$. Invoking Theorem 9.8.8(2) and Corollary 9.9.7, we get PST from $\mathbf{e}_u \otimes (\mathbf{e}_a + s\mathbf{e}_b)$ to $\mathbf{e}_v \otimes (\mathbf{e}_b + s\mathbf{e}_a)$ at time τ. Additionally, if $|s| = 1$, then (9.8.3) implies that we have PST from $\mathbf{e}_u \otimes (\mathbf{e}_a + s\mathbf{e}_b)$ to $\mathbf{e}_v \otimes (\mathbf{e}_a + \overline{s}\mathbf{e}_b)$ at time τ.

In particular, this example holds if we take $\tau = \frac{\pi}{2}$, $X = Q_d$ for $d \geq 3$ and Y be any graph that has vertex PST at $\pi/2$ (there are many such graphs, like some families of integer-weighted Hadamard diagonalisable graphs constructed in [60]).

10

Future work

In order to inspire further work on this topic, we provide a compilation of open questions motivated by the previous chapters in this thesis.

10.1 Periodicity

By Theorem 4.2.3, perfect state transfer between m-strongly cospectral pure states yields periodicity, and the minimum period of the pure states involved is m times the minimum PST time by Theorem 4.4.2(2). This leads us to our first problem.

Problem 1. Generate infinite families of unweighted graphs that admit perfect state transfer involving periodic pure states that are not m-strongly cospectral. How are the minimum PST time τ and minimum period ρ related for such pure states? Is ρ always an integer multiple of τ even if the pure states involved are not m-strongly cospectral?

10.2 Prescribed PST

In Theorem 4.6.3, we showed that for all $\mathbf{x}, \mathbf{y} \in \mathbb{C}^n$ that are linearly independent, for all $\tau > 0$, for all unit complex number γ and for all integers $2 \leq r \leq n$, there exists a Hermitian matrix M such that $|\Phi_{\mathbf{x}}| = r$ and perfect state transfer occurs from $\mathbf{x}$ to $\mathbf{y}$ at time τ with phase factor γ. Our proof relies on the existence of a unitary matrix that maps a given orthonormal basis to another. This guarantees the Hermiticity of M. In particular, if we take $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$, then Corollary 6.1.10 implies that M can be chosen to be real symmetric. This leads to the following question.

Problem 2. Refine the proof of Theorem 4.6.3 to produce a Hamiltonian M that has at least one of the following properties: irreducible, nonnegative, hollow and has integer entries. Is it possible to construct a matrix M that possess all these properties?

10.3 Time complexity

In [36], it was shown that for any $n \times n$ symmetric integer matrix M whose entries belong to $[-p(n), p(n)]$ for some polynomial $p(x)$, deciding whether perfect state transfer occurs between vertex states relative to M can be done in polynomial time in n. Such time complexity relies on the characterisation of perfect state transfer given in Corollary 6.1.9.

Now that we have the most general characterisation of perfect state transfer (see Theorem 4.1.3), we pose the following question.

Problem 3. For any $n \times n$ real symmetric matrix M, what additional conditions must we impose (either on M or on the pure states in question) to ensure that deciding whether perfect state transfer occurs from a pure state to another relative to M can be done in polynomial time in n? Is there a time complexity for s-pair states that is analogous to that of vertex states mentioned above?

10.4 s-pair state transfer

In Theorem 9.8.8, we characterised s-pair state transfer in distance-regular graphs with vertex PST whenever $s \in \mathbb{R}\backslash\{0\}$. These graphs are antipodal, and so we would like to investigate the following problem that complements our result.

Problem 4. Determine all occurrences of s-pair state transfer in antipodal distance-regular graphs that do not admit vertex PST whenever $s \in \mathbb{R}\backslash\{0\}$.

In Section 9.9 of Chapter 9, several constructions of perfect state transfer between an s- and an r-pair state where $|r| = |s|$ were given. In particular, we have examples where $r \in \{s, -s, \overline{s}\}$. Driven by our desire to see more examples of s-pair state transfer, we include the following problem.

Problem 5. Find new constructions of s- and r-pair states admitting perfect state transfer, where $|r| = |s|$ and $s \notin \mathbb{R}$. In particular, we are interested in knowing more examples for the case where $r \in \{s, -s, \overline{s}\}$.

We are also interested in the following problems.

Problem 6. Provide infinite families of unweighted graphs admitting perfect state transfer between an s- and an r-pair state, where $|r| \neq |s|$.

Problem 7. Provide infinite families of unweighted graphs where an s-pair state $\mathbf{e}_a + s\mathbf{e}_b$ admits perfect state transfer to two linearly independent r- and q-pair states $\mathbf{e}_u + r\mathbf{e}_v$ and $\mathbf{e}_x + q\mathbf{e}_y$ (possibly at different times).

Note that the above problem, s, r, and q are not all real. Otherwise, the three states involved are real, and the monogamy of perfect state transfer between real states (Theorem 6.1.2) implies that $\mathbf{e}_u + r\mathbf{e}_v$ and $\mathbf{e}_x + q\mathbf{e}_y$ are linearly dependent, a contradiction.

Trees are of great interest to physicists. However, trees in general do not admit vertex PST relative to A and L [40, 41]. Recently, a construction of Pal gave rise to infinite families of trees with maximum degree three admitting pair state transfer [80]. Hence, we would like to know if there are other values of s for which there is s-pair state transfer on trees. So we ask:

Problem 8. Characterise s-pair state transfer in trees for all $s \in \mathbb{R}$.

10.5 Graph operations

A *weak Hadamard matrix* H is a matrix with entries from the set $\{0, \pm 1\}$ such that $H^T H$ is tridiagonal. A graph X is *weakly Hadamard diagonalisable* (WHD) if its Laplacian matrix is diagonalisable by a weak Hadamard matrix. Note that a weak Hadamard matrix and a weakly Hadamard diagonalisable graph are generalisations of a Hadamard matrix and a Hadamard diagonalisable graph. Vertex PST was studied in WHD graphs [71]. In line with our result in Corollary 8.7.1, we ask:

Problem 9. When does a blow-up of a WHD graph admit PST?

Using edge perturbations, Theorem 8.9.2 outlines a way of inducing PST between non-adjacent twin vertices under mild conditions relative to L. This naturally leads to the following question.

Problem 10. Is there a result analogous to Theorem 8.9.2 relative to A? That is, if $n \equiv 0 \pmod 4$, will the addition of an appropriate matching in $\overset{n}{\uplus} X$ induce vertex PST relative to A?

If X is a weighted join graph with odd number of vertices and $\phi(L(X), t)$ has integer coefficients, then Corollary 7.3.3 implies that vertex PST does not occur in X. This is also known to be true for all unweighted graphs with $n \in \{3, 5\}$ vertices, which are not necessarily joins. Thus, we ask:

Problem 11. If X is a connected unweighted graph on an odd number of vertices, does vertex PST occur in X relative to L?

Since the join and the blow-up operation are able to produce graphs with vertex PST from graphs that do not have such a property, we are also interested in the following problem.

Problem 12. Suppose a graph X does not admit PST between any pair of vertices. What other graph operations can we perform on or with X that results in a larger graph that admits PST?

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