Quantum State Transfer in Graphs

by

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Author's Declaration

I hereby declare that I am the sole author of this thesis. This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

I understand that my thesis may be made electronically available to the public.

Abstract

Let X be a graph, A its adjacency matrix, and $t \in \mathbb{R}_{\geq 0}$. The matrix $\exp(\mathtt{i}tA)$ determines the evolution in time of a certain quantum system defined on the graph. It represents a continuous-time quantum walk in X. We say that X admits perfect state transfer from a vertex u to a vertex v if there is a time $\tau \in \mathbb{R}_{\geq 0}$ such that

$$\left| \exp(\mathtt{i}\tau A)_{u,v} \right| = 1.$$

The main problem we study in this thesis is that of determining which simple graphs admit perfect state transfer. For some classes of graphs the problem is solved. For example, P_n admits perfect state transfer if and only if $n = 2$ or $n = 3$. However, the general problem of determining all graphs that admit perfect state transfer is substantially hard.

In this thesis, we focus on some special cases. We provide necessary and sufficient conditions for a distance-regular graph to admit perfect state transfer. In particular, we provide a detailed account of which distance-regular graphs of diameter three do so.

A graph is said to be spectrally extremal if the number of distinct eigenvalues is equal to the diameter plus one. Distance-regular graphs are examples of such graphs. We study perfect state transfer in spectrally extremal graphs and explore rich connections to the topic of orthogonal polynomials. We characterize perfect state transfer in such graphs.

We also provide a general framework in which perfect state transfer in graph products can be studied. We use this to determine when direct products and double covers of graphs admit perfect state transfer. As a consequence, we provide many new examples of simple graphs admitting perfect state transfer. We also provide some advances in the understanding of perfect state transfer in Cayley graphs for ${\mathbb{Z}_2}^d$ and $\mathbb{Z}_n$.

Finally, we consider the problem of determining which trees admit perfect state transfer. We show more generally that, except for K_2, if a connected bipartite graph contains a unique perfect matching, then it cannot admit perfect state transfer. We also consider this problem in the context of another model of quantum walks determined by the matrix $\exp(\mathtt{i}tL)$, where L is the Laplacian matrix of the graph. In particular, we show that no tree on an odd number of vertices admits perfect state transfer according to this model.

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Chapter 1

Introduction

This thesis is about graph-theoretic problems motivated by quantum computing theory. A quantum bit, or a *qubit*, is a two-state quantum system, and as such it is the basic unit of quantum information. Our underlying assumption is that a graph represents a network of interacting qubits, and our main motivation is to understand how information flows in such a network accordingly to specified rules. The key concept is that of a continuous-time quantum walk, first introduced in 1998 by Farhi and Gutmann in [26] to develop quantum algorithms using decision trees. We however stress that despite the quantum flavoured motivation of our goals, this is a thesis in algebraic graph theory.

We will see that for a simple and natural choice of a time-independent Hamiltonian, the evolution of a state of the network of qubits depends uniquely on the spectral properties of the adjacency matrix of the underlying graph. This connection motivates the main goal of this thesis.

(1) Determine for which graphs the overlying network of qubits admits a perfect transfer of quantum state between two of its qubits.

The following secondary goals naturally arise from this quest.

(2) Understand the relation between classical graph properties and quantum motivated properties.

(3) Examine other distinguished quantum states that depend solely on spectral information of the graph.

(4) Examine another coupling model that is related to the Laplacian matrix of the graph.

We obtained partial success in all of the aforementioned goals. In the next section, we discuss some of the motivation to our research.

1.1 Motivation

To motivate the problem in this thesis, we introduce some definitions.

A qubit is the quantum analogue of a classical bit. Whereas a bit can take any value in the set $\{0, 1\}$, a qubit can be assigned to any 1-dimensional subspace from a 2-dimensional complex vector space. In this sense, we associate a qubit to such a 2-dimensional space, and a state of such a qubit to one of the 1-dimensional subspaces. Given a graph X with n vertices, we suppose that the vertices of the graph represent qubits, and that the edges represent quantum wires between such qubits. The energy of the system is expressed in terms of a Hermitian matrix H, called the Hamiltonian. We choose a time-independent Hamiltonian, and thus the Schrödinger equation of quantum mechanics will imply that the evolution of the system is governed by the matrix $\exp(-\mathtt{i}tH/\hbar)$, where t is a positive time and $\hbar$ is the Planck constant divided by 2π. We initialize our system setting a fixed qubit to a particular state, and all other qubits to the orthogonal state. The classical analogy would be to initialize one bit as 1, and all other bits as 0. With these settings, it turns out that the evolution of the system will be determined by a matrix of dimension n rather than 2^n.

Let X be a simple and undirected graph. By $A = A(X)$ we denote the symmetric matrix whose rows and columns are indexed by the vertices of X, and we fill this matrix with 1s whenever the corresponding vertices are adjacent, and 0 otherwise. This matrix is known as the adjacency matrix of X. If $D = D(X)$ is a diagonal matrix whose entries correspond to the degrees of the vertices of X, we define the Laplacian matrix $L = L(X)$ by $L = D - A$.

Upon certain choices of a time-independent Hamiltonian, more specifically the XY-coupling model or the XYZ-coupling model, the quantum system defined in the graph as above will evolve accordingly to $\exp(\mathtt{i}tA)$ or to $\exp(\mathtt{i}tL)$ respectively. The dynamics of the quantum states in each vertex resembles in some aspects the dynamics of a random walk. For instance, at each point in time, the squares of the absolute values of each entry of a column of $\exp(\mathtt{i}tA)$ determine a probability distribution on the vertices of X. For that reason, we typically say that such a matrix represents a continuous-time quantum walk on the graph. Note however that many intrinsic properties of classical random walks are not true for quantum walks. For example, there is no convergence to a uniform distribution; except in empty graphs, quantum walks always have an oscillatory behaviour.

The problem we are mostly concerned about is that of determining a time τ in which the quantum state input in a vertex is transferred with probability one to another vertex. Naturally, this would be related to the problem of transferring information in a quantum system with no errors. We formalize this below.

Let X be a graph on n vertices with adjacency matrix $A = A(X)$. Using the power series for the exponential function, we have

$$\exp(\mathtt{i}tA) = \sum_{k \geq 0} \frac{(\mathtt{i}t)^k}{k!} A^k.$$

Given two vertices u and v of X, we denote their respective characteristic vectors by $\mathbf{e}_u \in \mathbb{R}^n$ and $\mathbf{e}_v \in \mathbb{R}^n$. We say that X admits perfect state transfer (with respect to the XY-coupling model) from vertex u to vertex v at a time $\tau \in \mathbb{R}^+$ if there is a complex number λ such that

$$\exp(\mathtt{i}\tau A)\mathbf{e}_u = \lambda \mathbf{e}_v.$$

We say that X is periodic at u if $u = v$ in the equation above. Analogous definitions hold for the XYZ-coupling model, with L taking the place of A above.

Finding graphs that admit perfect state transfer with respect to these coupling models is therefore translated into a problem that depends uniquely on the spectral properties of the matrices A or L, and thus a problem in classical algebraic graph theory. This problem was first proposed by Christandl et al. in [19] and [20], and since then, it has received a considerable amount of attention from the physics and mathematics communities. In the last section of this chapter, we will review some of the work that has been done in the area.

The applicability of our findings faces major challenges, for instance, whether or nor a quantum computer will ever be built. For that reason, it is fair to say that our main motivation to work on this problem has a strong intrinsic aspect, influenced by our curiosity to understand how the spectral properties of graph correlate to other graph properties. More specifically, we will see that the questions raised by our investigation on the relationship between the spectral properties of a graph and quantum walks are new and interesting. We believe that these are questions that by themselves deserve attention, but we will try to keep in the back of our mind the potential applicability of our results in quantum computing. After all, mathematics is often motivated by goals even more abstract than ours, and yet there are countless examples of mathematical theories that find practical applications decades or even centuries after their development.

The following section contains an overview of our main results.

1.2 Overview of results

Let X be a simple undirected graph on n vertices and let $A = A(X)$ be its adjacency matrix. Suppose the set of distinct eigenvalues of A is equal to $\{\theta_0, ..., \theta_d\}$. The matrix A is symmetric, and therefore there exists an orthogonal basis of $\mathbb{R}^n$ consisting of eigenvectors of A. As a consequence, A admits a spectral decomposition into orthogonal projections given by

$$A = \sum_{r=0}^{d} \theta_r E_r.$$

A very important feature of this decomposition is that it allows for power series evaluated in A to be expressed as linear combinations of the projection matrices. More specifically, we have that

$$\exp(\mathtt{i}tA) = \sum_{r=0}^{d} \mathtt{e}^{\mathtt{i}t\theta_r} E_r.$$

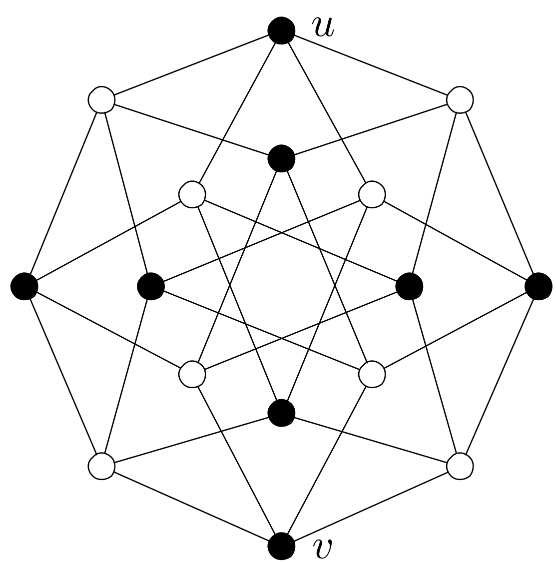
Because the projection matrices are orthogonal, that is, if $r \neq s$ then $E_r E_s = \mathtt{0}$, it follows that $\exp(\mathtt{i}tA)\mathbf{e}_u = \lambda \mathbf{e}_v$ if and only if, for all $r \in \{0, ..., d\}$, we have

$$\mathtt{e}^{\mathtt{i}t\theta_r} E_r \mathbf{e}_u = \lambda E_r \mathbf{e}_v.$$

As a consequence, for all r, the real vectors $E_r\mathbf{e}_u$ and $E_r\mathbf{e}_v$ must satisfy

$$E_r \mathbf{e}_u = \pm E_r \mathbf{e}_v. \tag{1.1}$$

Vertices u and v satisfying the condition above are called strongly cospectral. The existence of strongly cospectral vertices imposes significant restrictions on the structure of graphs that might admit perfect state transfer. The following graph is an example of a graph that contains pairs of strongly cospectral vertices. It is the skeleton of the 4-dimensional hypercube. The black vertices are those at even distance from u, and the white vertices are those at odd distance from u.



This graph satisfies the following three important properties.

(1) The number of edges from a vertex at distance i from u to the set of all vertices at distance j from u depends only on i and j. For example, all vertices at distance two from u have precisely two neighbours at distance three from u.

(2) Property (1) is valid if we replace u for any vertex w of the graph. Moreover, the number of edges from a vertex at distance i from w to the set of all vertices at distance j from w does not depend on the choice of w.

(3) For each vertex w of the graph, there is a unique vertex at maximum distance from w. For example, v is the unique vertex at distance four from u.

A partition of the vertex set of a graph according to the distance from a fixed vertex u is called the distance partition of u. If a distance partition satisfies property (1), it is called an equitable distance partition. The numbers of edges between the cells of the partition are known as the parameters of the partition.

Graphs satisfying properties (1) and (2) are called distance-regular. If a distance-regular graph satisfies property (3), then it is called an antipodal distance-regular graph with fibres of size two. When these graphs have diameter three, they correspond to rich combinatorial structures known as regular two-graphs.

The first more specific question that we addressed was to determine which distance-regular graphs admit perfect state transfer. We devote Chapter 3 to this topic. The most important result in this chapter is the following, which we use to completely determine which of the known distance-regular graphs admit perfect state transfer.

3.2.3 Theorem. *Suppose X is a distance-regular graph with distinct eigenvalues $\theta_0 > ... > \theta_d$. Then X admits perfect state transfer between vertices u and v if and only the following holds.*

(i) The eigenvalues of X are integers.

(ii) X is antipodal with fibres of size two, and u and v are antipodal vertices.

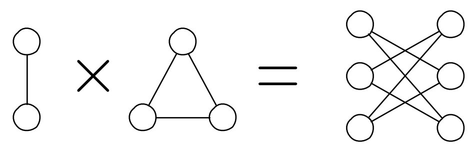
(iii) For all odd r, the power of two in the factorization of $\theta_0 - \theta_r$ is a constant, say α.

(iv) For all even r, the power of two in the factorization of $\theta_0 - \theta_r$ is larger than α.

As an application of the theorem above, we are able to completely characterize perfect state transfer in graphs corresponding to regular two-graphs (see Theorems 3.2.13 and 3.2.14, and Table 3.1).

An association scheme consists of a set of 01-matrices satisfying certain combinatorial properties that resemble the regularity properties observed in distance-regular graphs. The algebra spanned by these 01-matrices is called the Bose-Mesner algebra of the association scheme. We observed that the techniques we used to study perfect state transfer in distance-regular graphs could be applied to graphs whose adjacency matrix belongs to the Bose-Mesner algebra of an association scheme.

Let X and Y be graphs with adjacency matrices $A(X)$ and $A(Y)$. The direct product of X and Y, denoted by $X \times Y$, is the graph defined by the adjacency matrix $A(X \times Y) = A(X) \otimes A(Y)$. Observe the example below.



If X is a distance-regular graph, its direct product with K_2 is a graph whose adjacency matrix belongs to the Bose-Mesner algebra of an association scheme. Using this fact, we are able to find many new examples of perfect state transfer in simple graphs through the use of the following theorem.

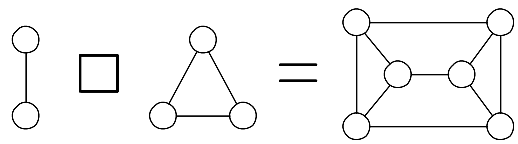
3.3.4 Theorem. *Let $V(K_2) = \{v_1, v_2\}$. Suppose X is distance-regular on n vertices with eigenvalues $\theta_0 > ... > \theta_d$, and let $\theta_r = 2^{f_r}\ell_r$, where ℓ_r is an odd integer. For any vertex $u \in V(X)$, the direct product $X \times K_2$ admits perfect state transfer between (u, v_1) and (u, v_2) if and only if both conditions below hold.*

(i) For all r, we have $f_r = a$ for some constant a.

(ii) For all r and s, we have $\ell_r \equiv \ell_s \bmod 4$.

We define below two other graph products which are objects of our study.

Let X and Y be graphs with adjacency matrices $A(X)$ and $A(Y)$. The Cartesian product of X and Y, denoted by $X \square Y$, is the graph defined by the adjacency matrix $A(X \square Y) = A(X) \otimes \mathtt{I} + \mathtt{I} \otimes A(Y)$. Observe the example below.

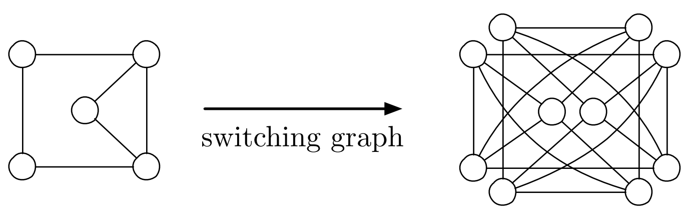


The n-th Cartesian power of X will be denoted by $X^{\square n}$.

If X and Y are graphs constructed on the same vertex set with n vertices, we define $X \ltimes Y$ as the graph with adjacency matrix

$$A(X \ltimes Y) = \begin{pmatrix} A(X) & A(Y) \\ A(Y) & A(X) \end{pmatrix}.$$

If X and Y do not contain a common edge, then $A(X) + A(Y)$ defines a graph. The graph $X \ltimes Y$ is double cover of the graph with adjacency matrix $A(X) + A(Y)$. If $\overline{X}$ denotes the complement of X, then $X \ltimes \overline{X}$ is a double cover of the complete graph on n vertices known as the switching graph of X.



Antipodal distance-regular graphs of diameter three and fibres of size two defined on n vertices are double covers of the complete graph K_n. Double covers and direct products with K_2 can both be studied within a much more general framework. We introduce this approach in Chapter 4, and we study perfect state transfer in this context. As a consequence, we are able to provide necessary and sufficient conditions for certain graph products to admit perfect state transfer, including double covers of the complete graph. The main contribution of this chapter comprises many new examples of perfect state transfer, which we find using the following two corollaries.

4.2.6 Corollary. *Suppose X and Y graphs. If Y admits perfect state transfer, if the eigenvalues of X and Y are integers or integer multiples of a square root, and if the powers* *of two in the factorization of the integer parts of the eigenvalues of X are all the same, then there exists a $k_0 \in \mathbb{Z}^+$ such that $X \otimes Y^{\square(mk_0)}$ admits perfect state transfer for all $m \geq 1$.*

4.4.4 **Corollary.** *Suppose X and Y are graphs on the same vertex set, and let u be a vertex of these graphs. Suppose $A(X)$ and $A(Y)$ commute. Then perfect state transfer happens in $X \ltimes Y$ between the two copies of u if and only if there is a time τ such that X is periodic at u at time τ, and Y is periodic at u at time τ and with phase $\pm\mathtt{i}$.*

We call a graph spectrally extremal if the number of distinct eigenvalues is equal to the diameter plus one. Given a vertex u of a graph X, its eccentricity is the maximum distance from u to any vertex of X. The eigenvalue support of u is the set of eigenvalues such that the projection of $\mathbf{e}_u$ onto the corresponding eigenspace is non-zero. A vertex is spectrally extremal if the size of its eigenvalue support is equal to its eccentricity plus one.

It turns out that spectral extremality is a concept with very interesting connections to the topics of equitable partitions and orthogonal polynomials. In the context of quantum walks, one of our most important results is an example of such relations. We say that u and v are (a pair of) antipodal vertices if the distance partition of u is equitable, $\{v\}$ is a singleton in the partition at maximum distance from u, and the parameters of the partition are symmetric with respect to u and v.

6.3.3 **Theorem.** *Suppose X is regular and 2-connected. Then u and v are antipodal vertices in X if and only if u and v are spectrally extremal and strongly cospectral to each other.*

We also study perfect state transfer in spectrally extremal graphs, and we find a generalization of our result for distance-regular graphs.

6.4.2 **Corollary.** *Suppose X is a spectrally extremal regular graph of diameter d on n vertices, having distinct eigenvalues $\theta_0 > ... > \theta_d$. Then X admits perfect state transfer between any two vertices u and v at distance d if and only if*

(i) All eigenvalues are integers.

(ii) For all odd r, the power of 2 in the factorization of $\theta_0 - \theta_r$ is a constant, say α.

(iii) For all even r, the power of 2 in the factorization of $\theta_0 - \theta_r$ is larger than α.

(iv) The following equality holds

$$n \prod_{s=0}^{d} \frac{1}{\theta_0 - \theta_s} = \sum_{r=0}^{d} (-1)^r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s}.$$

The last major problem we address in the thesis is that of determining which trees admit perfect state transfer. We will examine this problem with respect to the adjacency matrix and with respect to the Laplacian matrix. In the former case, we note that our observations are easily generalized to bipartite graphs in general. Our strongest result is the following.

7.1.4 Theorem. *Except for K_2, no connected bipartite graph with a unique perfect matching admits perfect state transfer.*

In the quantum model associated to the Laplacian matrix, we apply the Matrix-Tree Theorem to show the following result, which in particular shows that no tree on an odd number of vertices admits perfect state transfer in this model.

7.3.6 Theorem. *If X is a graph on an odd number of vertices with an odd number of spanning trees, then perfect state transfer with respect to the Laplacian cannot happen.*

The results above indicate that perfect state transfer is a rare phenomenon in trees, perhaps happening only on P_2 and P_3.

1.3 Brief literature review

A continuous-time quantum walk matrix was first considered by Farhi and Gutmann [26] in 1998, but in a context different than ours. Bose [11] in 2003 proposed a scheme for using spin chains to achieve the task of transmitting a quantum state. In [19], 2004, Christandl, Datta, Ekert and Landahl defined the problem of finding perfect state transfer in quantum spin networks with respect to the nearest-neighbour XY-coupling model. Since then, the topic has received a considerable amount of attention from the physics and mathematics communities. We summarize in the list below some of the major achievements in the problem of determining which undirected graphs admit perfect state transfer in the XY− or the XYZ-coupling models. Only for the list below, we will use *PST* to refer to perfect state transfer.

1) Christandl et al. [20]. Extends the work done in [19] by Christandl et al. They showed that if PST happens in graphs admitting mirror-symmetry, the ratio of certain differences of eigenvalues must be rational. They used this fact to show that PST does not happen in paths P_n for $n \geq 4$. To achieve PST at larger distances, they showed that if a graph admits PST, any iterated Cartesian power of itself also admits PST, and thus they examine powers of P_2 and P_3. They used that to show that weighted paths of arbitrary length may admit PST.

2) Kay [52] worked on the problem of transfer of state using other coupling models. In [51], he showed that if PST happens in a simple graph between two vertices, neither can be involved in PST with a third vertex.

3) Godsil [34] explored different aspects of state transfer. For instance, he showed that eigenvalues in the eigenvalue support of vertices involved in PST must be quadratic integers. He also considered the relation between PST and concepts such as controllable vertices, cospectral vertices and equitable partitions.

4) A Cayley graph on the group ${\mathbb{Z}_2}^d$ is called a cubelike graph. Bernasconi et al. [9] showed that if a cubelike graph is defined in terms of a connection set whose sum is not 0, then such graphs admit PST at time $\frac{\pi}{2}$. Cheung and Godsil [18] subsequently studied cubelike graphs whose connection set sum is 0. In that case, PST might or might not happen, and they provided necessary and sufficient conditions for PST that are stated in terms of a linear code associated to the graph. If PST happens in this case, it must be at a time $< \frac{\pi}{2}$.

5) A Cayley graph on the group $\mathbb{Z}_n$ is called a circulant graph. Saxena et al. [63] showed that any circulant graph admitting perfect state transfer must have integral eigenvalues (their argument was later extended to any regular graph). In a sequence of three papers, Bašić et al. ([7], [62] and [8]) provided necessary and sufficient conditions for circulant graphs to admit PST.

6) Some constructions using joins and products were studied by Tamon and other authors. Angeles-Canul et al. [3] showed that certain joins of regular graphs with K_2 or its complement admit PST. The same set of authors also studied weighted joins of graphs in [4]. Ge et al. [31] analysed some graph products and weighted joins. Finally, Bachman et al. [5] considered some asymmetric graphs admitting PST whose quotient is a weighted path.

7) Godsil [33] showed that if a graph whose adjacency matrix belongs to the Bose-Mesner algebra of an association scheme admits PST, then one of the classes of the scheme is a permutation matrix of order 2. He also studied walk-regular graphs in the context of state transfer. Coutinho et al. [21] extended that necessary condition to a set of sufficient conditions for graphs belonging to such algebras to admit PST, finding more examples of PST in simple graphs.

8) PST on distance-regular graphs had been previously considered by Jafarizadeh and Sufiani [48]. Together with other authors, they considered the problem of engineering the Hamiltonian to obtain PST on locally distance-regular graphs and group schemes (respectively [49] and [50]).

9) Vinet and Zhedanov ([67] and [66]) worked out some examples of PST on weighted paths based on the theory of orthogonal polynomials.

10) Some valuable surveys have been published in the past years. Kendon and Tamon [55] surveyed results about PST in join constructions, weighted paths and circulant graphs. They also discussed discrete-time quantum walks. Kay [53] reviewed the topic of PST, and proceeded to show how it can be used to achieve some features related to quantum computation. Godsil [39] reviewed some results on PST focusing on the algebraic graph theory behind the properties of $\exp(\mathtt{i}tA)$.

Chapter 2

Background

The purpose of this chapter is to provide sufficient background for all other chapters of this thesis. We will first introduce most of the graph-theoretic definitions and notation that we will use later on in this thesis. We will also state basic important theorems of linear algebra and algebraic graph theory. This section can be skipped by any reader familiar with the topic, and most, if not all of the material can be found in Godsil and Royle [42] and Brouwer and Haemers [14]. We will assume the reader is familiar with standard definitions related to graph theory. For that, our main reference is Bondy and Murty [10].

Following this, we will build the basic connection between continuous-time quantum walks and algebraic graph theory. Our main source for this section is Christandl et al. [20]. We will not aim to provide a self-contained introduction to quantum mechanics or quantum computing theory. For the former we suggest Hall [45], and for the latter we recommend Kaye et al. [54]. Section 2.3 contains a very short summary of the results from number theory and field theory that we will use throughout this thesis.

The final sections are dedicated to introducing the basic results about the main topic of this thesis. We will try our best to be self-contained, including all background material needed for future chapters. In this chapter, there are essentially no new results, but some ideas will be presented in a new and more useful form, and new proofs of some results are also included.

2.1 Algebraic graph theory

Here and throughout all of this thesis, unless otherwise explicitly stated, we will use the word "graph" to mean a finite, simple and undirected graph. The letters X and Y will always be used to represent graphs, and $V(X)$ and $E(X)$ will be respectively the vertex and edge set of X. We will reserve u, v, w, a and b for the vertices of our graphs, and our edges will always be represented as a pair of vertices. The *adjacency matrix* of a graph is the symmetric 01-matrix whose rows and columns are indexed by the vertices of the graph and whose entries are defined as follows

$$A(X)_{u,v} = \begin{cases} 1 & \text{if } uv \in E(X), \\ 0 & \text{otherwise.} \end{cases}$$

We stress here the chosen order of the vertices to index the rows and columns is not relevant, as long as we are consistent with it. Moreover, we have the following interpretation of the isomorphisms of a graph.

2.1.1 Lemma. *Graphs X and Y are isomorphic if and only if there is a permutation matrix P such that $P^T A(X) P = A(Y)$.*

When the context is clear, we shall denote $A = A(X)$. The powers of A provide information about the walks of X.

2.1.2 Lemma. *If $k \in \mathbb{N}$, then $(A^k)_{uv}$ is equal to the number of walks of length k whose end vertices are u and v.*

2.1.3 Corollary. *If $m = |E(X)|$, then $\operatorname{tr} A = 0$ and $\operatorname{tr} A^2 = 2m$.*

Throughout this thesis, we will usually denote the characteristic polynomial of $A(X)$ by $\phi_X(t)$. The eigenvalues of $A(X)$ will be referred to as the eigenvalues or the spectrum of the graph X. We will usually denote the distinct eigenvalues of X by θ_0, θ_1 etc.

The identity matrix of convenient order will be denoted by $\mathtt{I}$, the zero matrix by $\mathtt{0}$, and the all 1s matrix by $\mathtt{J}$. The all 1s vector will be denoted by $\mathbf{j}$, the zero vector by $\mathbf{0}$, and usually our vectors will receive bold letters. Given an ordering of the vertex set of X, usually that of the rows of $A(X)$, a vector of a standard basis corresponding to $u \in V(X)$ will be denoted by $\mathbf{e}_u$. For example, if $\overline{X}$ denotes the complement of X, note that

$$A(X) = \mathtt{J} - \mathtt{I} - A(\overline{X}).$$

The following theorem is one of the most important results of basic linear algebra.

2.1.4 Theorem. *A complex matrix M of order n is Hermitian if and only if there exists a basis of $\mathbb{C}^n$ consisting of orthonormal eigenvectors of M. Moreover, if M is Hermitian, all of its eigenvalues are real.*

A matrix E is called *idempotent* if $E^2 = E$. The following corollary will be referred to as the *spectral decomposition* a Hermitian matrix.

2.1.5 Corollary. *If $\{\theta_0, ..., \theta_d\}$ are the distinct eigenvalues of a Hermitian matrix M, then M can be written as*

$$M = \sum_{r=0}^{d} \theta_r E_r$$

where the matrices E_0,...,E_d satisfy

(1) E_r is an idempotent,

(2) $E_r E_s = \mathtt{0}$ if $r \neq s$,

(3) $\displaystyle\sum_{r=0}^{d} E_r = \mathtt{I}$.

Each of these matrices corresponds to an orthogonal projection onto the corresponding eigenspace.

The matrices E_r can be uniquely determined from the eigenvectors of M. If $\{\mathbf{v}_1, ..., \mathbf{v}_k\}$ is an orthonormal basis for the eigenspace associated to θ_r, then $E_r = \displaystyle\sum_{i=1}^{k} \mathbf{v}_i {\mathbf{v}_i}^*$.

If we are referring to an eigenvalue θ of a matrix M without the use of indices, we will use E_θ to denote the corresponding orthogonal projection. A very important feature of the decomposition above is the following theorem.

2.1.6 Theorem. *Suppose f is a univariate function and M is a Hermitian matrix with spectral decomposition $M = \sum_{r=0}^{d} \theta_r E_r$. If the Taylor series of f converges to f on the spectrum of M, then $f(M)$ is well defined in terms of the Taylor series of f, and moreover*

$$f(M) = \sum_{r=0}^{d} f(\theta_r) E_r.$$

2.1.7 Corollary. *If M has spectral decomposition $M = \sum_{r=0}^{d} \theta_r E_r$, then*

$$\langle \{M^k\}_{k \geq 0} \rangle = \langle E_r \rangle_{r=0}^{d}.$$

Proof. From Theorem 2.1.6, the powers of M can be written in terms of the E_r. But also if $p(x)$ is a polynomial such that $p(\theta_r) = 1$ and $p(\theta_s) = 0$ for all $s \neq r$, then $p(M) = E_r$, so the equality holds. □

The following theorem is a typical exercise in linear algebra textbooks, but will be very useful to us.

2.1.8 Theorem. *Symmetric matrices $M_1, ..., M_k$ of order n pairwise commute if and only if there exists one basis of $\mathbb{R}^n$ consisting of orthogonal eigenvectors for all of the matrices.*

The following result is usually referred to as the Perron-Frobenius Theorem. It can be presented in a more general framework, but here we will restrict to our needs.

2.1.9 Theorem. *Suppose X is a connected graph, and $A = A(X)$. Let θ_0 be the largest eigenvalue of A. Then the following properties hold.*

(1) The multiplicity of θ_0 is equal to one.

(2) There exists a strictly positive vector $\boldsymbol{v}$ such that $A\boldsymbol{v} = \theta_0 \boldsymbol{v}$.

(3) Any non-negative eigenvector of A belongs to the eigenspace of θ_0.

(4) If Y is a subgraph of X and σ is an eigenvalue of Y, then $|\sigma| \leq \theta_0$. Equality holds if and only if $Y = X$.

The largest eigenvalue of the graph will be referred to as the *Perron eigenvalue*, and the unique (up to scalar) positive eigenvector in its eigenspace will be called the *Perron eigenvector*.

2.1.10 Corollary. *A connected graph X is k-regular if and only if its Perron eigenvector is $\boldsymbol{j}$. In that case, the Perron eigenvalue is k.*

2.1.11 Corollary. *If X is a k-regular graph on n vertices, then $A(X)$ and $A(\overline{X})$ commute. Hence they can be simultaneously diagonalized, and if $\{k, \theta_1, ..., \theta_d\}$ are the distinct eigenvalues of X, the distinct eigenvalues of $\overline{X}$ are $\{(n-1-k),\ (-1-\theta_1),\ ...,\ (-1-\theta_d)\}$.*

For bipartite graphs, we have the following spectral characterization.

2.1.12 Theorem. *A connected graph X is bipartite if and only if $-\theta_0$ is an eigenvalue. In that case, for all eigenvalues θ of X, $-\theta$ is also an eigenvalue. Moreover, if $(\boldsymbol{v}_1, \boldsymbol{v}_2)$ is an eigenvector for θ partitioned according to the classes of X, then $(\boldsymbol{v}_1, -\boldsymbol{v}_2)$ is an eigenvector for $-\theta$.*

Finally, we present a theorem usually referred to as *interlacing*. If M is a symmetric matrix of order n, we denote by $\theta_1(M) \geq \theta_2(M) \geq ... \geq \theta_n(M)$ the eigenvalues of M.

2.1.13 Theorem. *If A is a symmetric matrix of order n, and B is a principal submatrix of A of order m, then, for $i = 1, ..., m$,*

$$\theta_{n-m+i}(A) \leq \theta_i(B) \leq \theta_i(A).$$

The obvious interpretation of the theorem above is that the eigenvalues of any induced subgraph of X interlace those of X.

2.2 Continuous-time quantum walks

In this section we address the problem of creating a quantum channel to transmit a quantum state from one location to another. To achieve that, we consider the quantum spin system model, where qubits are placed in a network whose dynamics is governed by a chosen Hamiltonian. Communication between qubits can be controlled in different ways, but here we will require a system with no external control. More specifically, after the network is manufactured, the evolution of the system depends uniquely on the initial state and on the structure of the network. Our goal is then to construct networks whose structure forces a perfect state transfer, that is, a transfer of state with probability 1. The main sources for this section are Christandl et al., [19] and [20]. This thesis is independent of this section, so it can be skipped without prejudice.

At this point, to maintain the consistency with the other parts of this text, we make the hard choice of avoiding the Dirac bra-ket notation.

Let X be a graph on n vertices, and to each vertex $u \in V(X)$ we assign a qubit, that is, a two-dimensional complex vector space $\mathcal{H}_u \simeq \mathbb{C}^2$. So the graph is associated to a space isomorphic to $\mathbb{C}^{2^n}$. We will denote the standard basis vectors of $\mathbb{C}^2$ by $\mathbf{f}_0$ and $\mathbf{f}_1$. For any $S \subset V(X)$, we denote

$$\mathbf{w}_S = \bigotimes_{u \in V(X)} \mathbf{f}_{i(u)}, \text{ where } \begin{cases} i(u) = 1 & \text{if } u \in S, \\ i(u) = 0 & \text{otherwise.} \end{cases}$$

Consider the Pauli matrices

$$\sigma^x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^y = \begin{pmatrix} 0 & -\mathtt{i} \\ \mathtt{i} & 0 \end{pmatrix}, \quad \sigma^z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

For a given ordering of the rows of $A(X)$, and $u \in V(X)$, we define

$$\sigma^x_u = \mathtt{I}_2 \otimes \cdots \otimes \mathtt{I}_2 \otimes \underbrace{\sigma^x}_{u\text{th position}} \otimes \mathtt{I}_2 \otimes \cdots \otimes \mathtt{I}_2,$$

where the product contains n multiplicands. We also consider analogous definitions for σ^y and σ^z.

We introduce two possible choices for a time-independent Hamiltonian.

$$H_{xy} = \frac{1}{2} \sum_{uv \in E(X)} J_{uv} \left(\sigma_u^x \sigma_v^x + \sigma_u^y \sigma_v^y \right), \quad \text{and} \tag{2.1}$$

$$H_{xyz} = \frac{1}{2} \sum_{uv \in E(X)} J_{uv} \left(\sigma_u^x \sigma_v^x + \sigma_u^y \sigma_v^y + \sigma_u^z \sigma_v^z - \mathtt{I}_{2^n} \right). \tag{2.2}$$

We choose the first and suppose $J_{uv} = 1$ for all $uv \in E(X)$, and denote $H = H_{xy}$. The Schrödinger Equation implies that if ϕ_0 is the initial state of the system, then the state ϕ at time t will be

$$\phi(t) = \mathtt{e}^{-\mathtt{i}tH/\hbar} \, \phi_0 \tag{2.3}$$

where $\hbar = \frac{h}{2\pi}$, and h is the Planck constant.

For $S, T \subset V(X)$, let $S \oplus T$ denote the symmetric difference of S and T. For any $S \subset V(X)$ and $uv \in E(X)$, we observe that

$$\frac{1}{2} \left(\sigma_u^x \sigma_v^x + \sigma_u^y \sigma_v^y \right) \mathbf{w}_S = \begin{cases} \mathbf{w}_{S \oplus \{u,v\}} & \text{if } |S \cap \{u,v\}| = 1, \\ 0 & \text{otherwise.} \end{cases} \tag{2.4}$$

Thus

$$H \mathbf{w}_S = \sum_{\substack{T \subset V(X) \\ |T| = |S| \\ S \oplus T \in E(X)}} \mathbf{w}_T. \tag{2.5}$$

Restricting to the case where $S = \{u\}$ for some $u \in V(X)$, and denoting $\mathbf{w}_{\{v\}} = \mathbf{w}_v$ for all $v \in V(X)$, we have

$$H \mathbf{w}_u = \sum_{uv \in E(X)} \mathbf{w}_v. \tag{2.6}$$

Hence the action of H on the subspace of $\mathbb{C}^{2^n}$ spanned by $\{\mathbf{w}_u\}_{u \in V(X)}$ is equivalent to the action of A on $\mathbb{C}^n$.

Now recall that we are motivated by the problem of transferring a quantum state from one qubit to another. By Equation 2.3, we say that the quantum system defined on X

admits *perfect state transfer* from vertex u to vertex v with respect to the XY-coupling model if, for some $\tau \in \mathbb{R}^+$ and $\lambda \in \mathbb{C}$, we have

$$\mathrm{e}^{-\mathrm{i}\tau H/\hbar}\ \mathbf{w}_u = \lambda \mathbf{w}_v. \tag{2.7}$$

Note that for the sake of studying perfect state transfer, we can conjugate on both sides and hence the sign on the exponent is irrelevant. We will also omit the constant $\hbar$, supposing it is absorbed by τ. Thus, by Equation 2.6, the quantum system on X admits perfect state transfer from u to v if and only if, for some $\tau \in \mathbb{R}^+$ and $\lambda \in \mathbb{C}$, we have

$$\mathrm{e}^{\mathrm{i}\tau A}\ \mathbf{e}_u = \lambda \mathbf{e}_v.$$

The analogy between a probability distribution on the vertex set of the graph determining quantum state transfer and a classical random walk in the graph is evident. For that reason, we will say that the matrix $\mathrm{e}^{\mathrm{i}tA}$ represents a model of a *continuous-time quantum walk* in X.

Let $D = D(X)$ be the diagonal matrix whose entries are the degrees of the corresponding vertices of X. The *Laplacian matrix* $L = L(X)$ is defined by $L = D - A$. By choosing the Hamiltonian $H = H_{xyz}$ from Equation 2.2, state transfer would be equivalent to

$$\mathrm{e}^{\mathrm{i}\tau L}\ \mathbf{e}_u = \lambda \mathbf{e}_v. \tag{2.8}$$

Most of this thesis is concerned with the Hamiltonian H_{xy}. We will address the Laplacian matrix case in Chapter 7.

2.3 Number theory and field theory

This short section contains a compilation of the definitions and results related to number theory and field theory that we will use in the thesis. Our main sources are Hardy and Wright [47] and Cox [22].

Definition. A real number μ is an *algebraic number* if it is the root of a polynomial $p(x)$ with integer coefficients, and it is an *algebraic integer* if that polynomial is monic.

Let $\mathbb{Q}[x_1, ..., x_n]$ denote the ring of all finite sums of monomials on the elements $\{x_1, ..., x_n\}$ with coefficients from $\mathbb{Q}$. By $\mathbb{Q}(x_1, ..., x_n)$ we denote the field of all rational functions on the elements $\{x_1, ..., x_n\}$. It is precisely the field of fractions of $\mathbb{Q}[x_1, ..., x_n]$. It follows that $\mathbb{Q}[x_1, ..., x_{n-1}][x_n] \cong \mathbb{Q}[x_1, ..., x_n]$, and analogously for $\mathbb{Q}(\cdot)$.

If $n = 1$ and $x_1 = x$ is algebraically independent over $\mathbb{Q}$, then $\mathbb{Q}[x]$ is precisely the ring of polynomials with rational coefficients. The *minimal polynomial* of an algebraic number μ is the monic polynomial $p(x) \in \mathbb{Q}[x]$ of minimal degree such that $p(\mu) = 0$. It follows that $p(x)$ cannot have non-trivial factors, and so it must be an irreducible polynomial. The *algebraic conjugates* of an algebraic number μ are the other roots of its minimal polynomial.

First, note the relation below. If μ is an algebraic number with minimal polynomial $p(x)$, and if $\langle p(x) \rangle$ denotes the ideal generated by $p(x)$, we have

$$\mathbb{Q}[\mu] \cong \mathbb{Q}[x]/\langle p(x) \rangle.$$

Note that $\mathbb{Q}$ is a field, hence $\mathbb{Q}[x]$ is a principal ideal domain and thus the ideal generated by irreducible elements is maximal. The quotient of a ring by a maximal ideal is a field, and therefore we have

$$\mathbb{Q}[\mu] \cong \mathbb{Q}(\mu).$$

Given a polynomial $p(x) \in \mathbb{Q}[x]$ of degree n whose set of roots over $\mathbb{C}$ is $\{\mu_1, ..., \mu_n\}$, this shows that $\mathbb{Q}[\mu_1, ..., \mu_n]$ is a field extension of $\mathbb{Q}$ that contains all roots of $p(x)$, and in fact, it is minimal with this property. It is called the *splitting field* of $p(x)$ over $\mathbb{Q}$.

We will be interested in two properties of the automorphisms of a splitting field.

2.3.1 Theorem. *If σ is an automorphism of any field extension of $\mathbb{Q}$, and if $p(x)$ is a polynomial with integer coefficients, then σ fixes the set of roots of $p(x)$ in this field extension.*

As a consequence, it follows that any automorphism of any extension of $\mathbb{Q}$ acts as the identity in $\mathbb{Q}$. A theorem due to Galois implies that this is actually a characterization.

2.3.2 Theorem. *Let $\mu \in \mathbb{Q}[\mu_1, ..., \mu_n]$. Then μ is fixed by all automorphisms of $\mathbb{Q}[\mu_1, ..., \mu_n]$ if and only if $\mu \in \mathbb{Q}$.*

In this thesis, we will be concerned with the algebraic numbers which are eigenvalues of integer matrices. Because the characteristic polynomial of a matrix is always monic with integer coefficients, the eigenvalues of an integer matrix are always algebraic integers. For that reason, we now move to focus on algebraic integers inside the extension field of $\mathbb{Q}$.

Let $\mathbb{Z}[x]$ denote the ring of polynomials with integer coefficients. If μ is an algebraic integer with minimal polynomial $p(x)$, it follows that

$$\mathbb{Z}[\mu] \cong \mathbb{Z}[x]/\langle p(x)\rangle.$$

Hence for any algebraic conjugate μ' of μ, we have

$$\mathbb{Z}[\mu] \cong \mathbb{Z}[\mu'].$$

As a consequence, we have the following proposition.

2.3.3 Proposition. *Let μ be an algebraic integer, μ' one of its conjugates, and σ be an isomorphism $\mathbb{Z}[\mu] \to \mathbb{Z}[\mu']$. If M is an integer-valued matrix with eigenvalue μ and a corresponding eigenvector $\boldsymbol{v}$, it follows that μ' is an eigenvalue of M with corresponding eigenvector $\sigma(\boldsymbol{v})$, with the understanding that σ is applied entry-wise.*

Definition. An algebraic integer μ whose minimal polynomial has degree two is called a *quadratic integer*.

The following characterization of quadratic integers may as well be considered folklore. It was originally given by Dedekind in his supplements of lectures by Dirichlet (see [25]).

2.3.4 Theorem. *A real number μ is a quadratic integer if and only if there are integers a, b and Δ such that Δ is square-free and one of the following cases holds.*

(i) $\mu = a + b\sqrt{\Delta}$ *and* $\Delta \equiv 2, 3 \pmod 4$.

(ii) $\mu = \frac{1}{2}\big(a + b\sqrt{\Delta}\big)$, $\Delta \equiv 1 \pmod 4$, *and either a and b are both even or both odd.*

Proof. If (i) holds, then μ is a solution to $x^2 - 2ax + (a^2 - b^2\Delta) = 0$. If (ii) holds, then μ is a solution to $x^2 - ax + \frac{1}{4}(a^2 - b^2\Delta) = 0$ and $\frac{1}{4}(a^2 - b^2\Delta) \in \mathbb{Z}$. In any case, μ is a quadratic integer.

Now let $x^2 + Ax + B = 0$ be the quadratic equation satisfied by μ. Note that $B \neq 0$. Let $a = -A$ and $b\sqrt{\Delta} = \sqrt{A^2 - 4B}$. From the quadratic formula, it follows that

$$\frac{1}{4}\big(a + b\sqrt{\Delta}\big)\big(a - b\sqrt{\Delta}\big) = B \in \mathbb{Z},$$

and hence

$$a^2 \equiv b^2\Delta \pmod 4.$$

If $\Delta \equiv 2, 3 \pmod 4$, a and b must be even, and so $\mu = a' \pm b'\sqrt{\Delta}$ for some $a', b' \in \mathbb{Z}$. If $\Delta \equiv 1 \pmod 4$, it could be the case that $a^2 \equiv b^2 \equiv 1 \pmod 4$, but in this case both a and b are odd. $\square$

We end this section introducing a notation that will be very useful throughout this thesis.

Definition. Given a rational number $\frac{a}{b}$ with a and b coprime, and given a prime p, if e is the largest integer such that p^e divides a, then the *p-adic norm* of $\frac{a}{b}$ is defined as

$$\left|\frac{a}{b}\right|_p = p^{-e}.$$

Note for example that if the power of 2 in the factorization of an integer a is larger than the power of 2 in the factorization of an integer b, then $|a|_2 < |b|_2$.

2.4 Perfect state transfer

Let M be a Hermitian matrix. For every non-negative real number t, we denote

$$U_M(t) = \exp(\mathtt{i}tM) = \sum_{k \geq 0} \frac{(\mathtt{i}t)^k}{k!} M^k. \tag{2.9}$$

We will omit the subscript M whenever the context is clear. Note that $U(0) = \mathtt{I}$ and $U(t_1 + t_2) = U(t_1)U(t_2)$. The matrix $U(t)$ is symmetric, and $U(-t) = \overline{U(t)}$, hence $U(t)$ is a unitary operator:

$$U(t)^*\, U(t) = \mathtt{I}. \tag{2.10}$$

Definition. We say that the Hermitian matrix M admits *perfect state transfer* from a column index u to a column index v if there exists a time $\tau \in \mathbb{R}^+$ and $\lambda \in \mathbb{C}$, called the *phase*, such that

$$U(\tau)\mathbf{e}_u = \lambda \mathbf{e}_v$$

Definition. We say that the Hermitian matrix M is *periodic* at a column index u if there is a time $\tau \in \mathbb{R}^+$ and phase $\lambda \in \mathbb{C}$ such that

$$U(\tau)\mathbf{e}_u = \lambda \mathbf{e}_u.$$

Because $U(t)$ is unitary, in both cases we must have $|\lambda| = 1$. We will use the properties of the proposition below without reference throughout the thesis.

2.4.1 Proposition. *If M admits perfect state transfer from u to v at time τ with phase λ, then*

(i) M admits perfect state transfer from v to u at the same time with the same phase.

(ii) M is periodic at both u and v at time 2τ and with phase λ^2.

Proof. By definition, $U(\tau)\mathbf{e}_u = \lambda \mathbf{e}_v$. Conjugating on both sides, we obtain

$$U(-\tau)\mathbf{e}_u = \overline{\lambda}\mathbf{e}_v,$$

and thus, since $\overline{\lambda} = \dfrac{1}{\lambda}$,

$$U(\tau)\mathbf{e}_v = \lambda \mathbf{e}_u.$$

As a consequence, we have $U(\tau)U(\tau)\mathbf{e}_u = \lambda U(\tau)\mathbf{e}_v$, and therefore

$$U(2\tau)\mathbf{e}_u = \lambda^2 \mathbf{e}_v.$$

□

The result above allows us to talk about perfect state transfer between indices u and v, instead of from u to v.

If X is a simple graph, the adjacency matrix $A = A(X)$ is Hermitian. Whenever we refer to the matrix $U(t)$ relative to X, we mean $U_A(t)$. By perfect state transfer in X between vertices u and v, we mean perfect state transfer in A between the column indices corresponding to u and v, and analogously for periodicity. Most of this thesis is concerned with this case, but in Chapter 7, we will study perfect state transfer with respect to the Laplacian matrix of X.

Example 1. If $X = K_2$, then note that $A^k = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ if k is even, and $A^k = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ if k is odd. Hence

$$\begin{aligned} U(t) &= \sum_{k \geq 0} (-1)^k \frac{t^{2k}}{(2k)!} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \mathtt{i} \sum_{k \geq 0} (-1)^k \frac{(t)^{2k+1}}{(2k+1)!} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \\ &= \begin{pmatrix} \cos(t) & \mathtt{i}\sin(t) \\ \mathtt{i}\sin(t) & \cos(t) \end{pmatrix}. \end{aligned}$$

Setting $t = \frac{\pi}{2}$, then it follows that

$$U\left(\frac{\pi}{2}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \mathtt{i} \begin{pmatrix} 0 \\ 1 \end{pmatrix}.$$

Hence K_2 admits perfect state transfer between its vertices at time $\frac{\pi}{2}$ and phase $\mathtt{i}$. □

The powers of an adjacency matrix are periodic if and only if the graph is a disjoint union of copies of K_2. So for other graphs, we need a different tool to study perfect state transfer.

Suppose that the Hermitian matrix M has distinct eigenvalues $\theta_0 > \theta_1 > ... > \theta_d$. By the Spectral Decomposition 2.1.5, we have

$$M = \sum_{r=0}^{d} \theta_r E_r.$$

By Theorem 2.1.6, it follows that

$$U(t) = \sum_{r=0}^{d} \mathtt{e}^{\mathtt{i}t\theta_r} E_r. \tag{2.11}$$

Example 2. Suppose $X = K_3$. Its eigenvalues are 2, -1 and -1, with corresponding orthogonal idempotents

$$\frac{1}{3}\begin{pmatrix}1 & 1 & 1\\ 1 & 1 & 1\\ 1 & 1 & 1\end{pmatrix} \quad \text{and} \quad \frac{1}{3}\begin{pmatrix}2 & -1 & -1\\ -1 & 2 & -1\\ -1 & -1 & -2\end{pmatrix}.$$

Hence

$$U(t)\begin{pmatrix}1\\0\\0\end{pmatrix} = \frac{1}{3}\begin{pmatrix}\mathrm{e}^{2\mathrm{i}t} + 2\mathrm{e}^{-\mathrm{i}t}\\ \mathrm{e}^{2\mathrm{i}t} - \mathrm{e}^{-\mathrm{i}t}\\ \mathrm{e}^{2\mathrm{i}t} - \mathrm{e}^{-\mathrm{i}t}\end{pmatrix}.$$

So the first vertex of K_3 is periodic at time $t = \frac{2\pi}{3}$, but is not involved in perfect state transfer with any of the other vertices. □

Definition. Given a Hermitian matrix M with spectral decomposition $M = \sum_{r=0}^{d} \theta_r E_r$ and a column index u of M, we say that an eigenvalue θ_r is in the *eigenvalue support* of u if $E_r \mathbf{e}_u \neq \mathbf{0}$. We will denote the eigenvalue support of u by Φ_u.

Example 3. The spectral decomposition of $A(P_3)$ is given by

$$A(P_3) = (\sqrt{2})\frac{1}{4}\begin{pmatrix}1 & \sqrt{2} & 1\\ \sqrt{2} & 2 & \sqrt{2}\\ 1 & \sqrt{2} & 1\end{pmatrix} + (0)\frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0 & -1\\ 0 & 0 & 0\\ -1 & 0 & 1\end{pmatrix} + (-\sqrt{2})\frac{1}{4}\begin{pmatrix}1 & -\sqrt{2} & 1\\ -\sqrt{2} & 2 & -\sqrt{2}\\ 1 & -\sqrt{2} & 1\end{pmatrix}$$

The eigenvalue support of the middle vertex is equal to $\{\sqrt{2}, -\sqrt{2}\}$, whereas the eigenvalue support of the other vertices is equal to $\{\sqrt{2}, 0, -\sqrt{2}\}$. □

If M is a Hermitian matrix, u a column index of M, it follows from Equation 2.11 that

$$U(t)\mathbf{e}_u = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} E_r \mathbf{e}_u,$$

and so M admits perfect state transfer between indices u and v at time τ and phase λ if and only if

$$\sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}\tau\theta_r} E_r \mathbf{e}_u = \lambda \mathbf{e}_v = \lambda \sum_{r=0}^{d} E_r \mathbf{e}_v,$$

where the last equality is a consequence of Corollary 2.1.5. Because the matrices E_r are orthogonal projectors, the equality above is true if and only if, for all $r = 0, ..., d$, we have

$$\mathtt{e}^{\mathtt{i}\tau\theta_r} E_r \mathbf{e}_u = \lambda E_r \mathbf{e}_v. \tag{2.12}$$

The numbers $\mathtt{e}^{\mathtt{i}\tau\theta_r}$ and λ are complex numbers of norm 1, and the vectors $E_r\mathbf{e}_u$ and $E_r\mathbf{e}_v$ are real, thus Equation 2.12 implies that

$$E_r \mathbf{e}_u = \pm E_r \mathbf{e}_v. \tag{2.13}$$

This equation motivates the definition below.

Definition. Given a Hermitian matrix M with spectral decomposition $M = \sum_{r=0}^{d} \theta_r E_r$ and column indices u and v of M, we say that u and v are *strongly cospectral* if, for all $r \in \{0, ..., d\}$,

$$E_r \mathbf{e}_u = \pm E_r \mathbf{e}_v.$$

Note that a trivial consequence of strong cospectrality is that $\Phi_u = \Phi_v$.

Definition. For any pair of column indices u and v of a Hermitian matrix M, let $\Phi_{uv}^{+} \subset \Phi_u$ be such that $\theta \in \Phi_{uv}^{+}$ if and only if $E_\theta \mathbf{e}_u = E_\theta \mathbf{e}_v$, and let Φ_{uv}^{-} be such that $\theta \in \Phi_{uv}^{-}$ if and only if $E_\theta \mathbf{e}_u = -E_\theta \mathbf{e}_v$.

Note that u and v are strongly cospectral if and only if $\Phi_{uv}^{+} \cup \Phi_{uv}^{-} = \Phi_u = \Phi_v$.

Unless otherwise stated, whenever we refer to the partition defined above or the terms eigenvalue support and strongly cospectrality in the context of a graph X and its vertices, we mean to use these definitions with respect to the adjacency matrix $A = A(X)$. The next section will be dedicated to study more properties of strongly cospectral vertices.

For a connected graph X, if u and v are strongly cospectral vertices, it follows from the Perron-Frobenius Theory 2.1.9 that the largest eigenvalue always belongs to Φ_{uv}^{+}; in our convention, $\theta_0 \in \Phi_{uv}^{+}$. Following up on the discussion above, we present a basic but important characterization of perfect state transfer.

2.4.2 Theorem. *Let X be a graph, $u, v \in V(X)$. Perfect state transfer between u and v occurs at time τ with phase λ if and only if all of the following conditions hold.*

(a) Vertices u and v are strongly cospectral.

(b) For all $\theta_r \in \Phi_{uv}^+$, there is a k such that $\tau(\theta_0 - \theta_r) = 2k\pi$.

(c) For all $\theta_r \in \Phi_{uv}^-$, there is a k such that $\tau(\theta_0 - \theta_r) = (2k+1)\pi$.

Given these conditions, $\lambda = \mathrm{e}^{\mathrm{i}\tau\theta_0}$.

Proof. From the implication Equation 2.12 $\implies$ Equation 2.13, we see that (a) is a necessary condition.

Now suppose u and v are strongly cospectral vertices. It follows from Equation 2.12 that perfect state transfer between u and v occurs if and only if there is a $\lambda \in \mathbb{C}$ such that $\mathrm{e}^{\mathrm{i}\tau\theta_r} = \pm\lambda$ for all r. Given that $\theta_0 \in \Phi_{uv}^+$, this is equivalent to

$$\begin{aligned} \mathrm{e}^{\mathrm{i}\tau\theta_0} &= \mathrm{e}^{\mathrm{i}\tau\theta_r} \quad \text{whenever } \theta_r \in \Phi_{uv}^+, \quad \text{and} \\ \mathrm{e}^{\mathrm{i}\tau\theta_0} &= -\mathrm{e}^{\mathrm{i}\tau\theta_r} \quad \text{whenever } \theta_r \in \Phi_{uv}^-. \end{aligned}$$

This is equivalent to, for some values of $k \in \mathbb{Z}$ depending on r,

$$\begin{aligned} \tau(\theta_0 - \theta_r) &= 2k\pi \quad \text{whenever } \theta_r \in \Phi_{uv}^+, \quad \text{and} \\ \tau(\theta_0 - \theta_r) &= (2k+1)\pi \quad \text{whenever } \theta_r \in \Phi_{uv}^-. \end{aligned} \tag{2.14}$$

□

The following theorem specifies which algebraic integers can be in the support of a periodic vertex.

2.4.3 Theorem (Godsil [34], Theorem 6.1)**.** *Suppose M is an integer Hermitian matrix. Then M is periodic at a column index u if and only if either of the following holds.*

(i) All of the eigenvalues in Φ_u are integers.

(ii) All but at most one of the eigenvalues in Φ_u are quadratic integers, and moreover, there is a square-free integer $\Delta > 1$ such that either

a) all the elements in Φ_u are integer multiples of $\sqrt{\Delta}$, or

b) there is an integer $a \neq 0$ such that every $\theta_r \in \Phi_u$ is of the form $\frac{1}{2}\big(a + b_r\sqrt{\Delta}\big)$ for integers b_r.

Proof. If (i) holds, take $\tau = 2\pi$, and if (ii) holds, take $\tau = \frac{2\pi}{\sqrt{\Delta}}$. In either case, τ is a time in which M is periodic at u.

Now we show that the conditions are necessary. Suppose θ_1 is an eigenvalue in the support of u which is not an integer, so that (i) does not hold. Let $\{\theta_2, ..., \theta_k\}$ be the set of algebraic conjugates of θ_1. All these numbers are eigenvalues of X, and by Proposition 2.3.3, these eigenvalues must be in the support of u. If M is periodic at u at time τ, it follows that $\mathrm{e}^{\mathrm{i}\tau\theta_i} = \mathrm{e}^{\mathrm{i}\tau\theta_j}$ for all $i, j \in \{1, ..., k\}$. As a consequence, $\tau(\theta_i - \theta_j)$ is always an integer multiple of π, and thus, for all $i, j \in \{1, ..., k\}$, we have

$$\frac{\theta_1 - \theta_2}{\theta_i - \theta_j} = \ell_{i,j} \in \mathbb{Q}.$$

Therefore

$$(\theta_1 - \theta_2)^{k(k-1)} = \prod_{i \neq j} \ell_{i,j}(\theta_i - \theta_j).$$

By Theorem 2.3.1, any field automorphism of $\mathbb{Q}[\theta_1, ..., \theta_k]$ fixes the set $\{\theta_1, ..., \theta_k\}$, and so fixes the right hand side of the equation above. Thus Theorem 2.3.2 implies that $(\theta_1 - \theta_2)^{k(k-1)}$ is a rational number, and because both θ_1 and θ_2 are algebraic integers, it follows that $(\theta_1 - \theta_2)^{k(k-1)} \in \mathbb{Z}$.

Let m be the smallest integer such that $(\theta_1 - \theta_2)^m = q \in \mathbb{Z}$. Note that any permutation of the set $\{\theta_1, \theta_2, ..., \theta_k\}$ provides a field automorphism of $\mathbb{Q}[\theta_1, ..., \theta_k]$, hence if $(\theta_1 - \theta_2)$ satisfies the equation $x^m - q = 0$, so does $(\theta_i - \theta_j)$ for all $i, j \in \{1, ..., k\}$. However at most two roots of $x^m - q$ are real, whereas all elements of $\mathbb{Q}[\theta_1, ..., \theta_k]$ are real. This implies that $k = 2$, and therefore all eigenvalues in the support of u which are not integers must be quadratic integers.

Now suppose at least one eigenvalue θ_1 in the support of u is a quadratic integer in $\mathbb{Q}(\sqrt{\Delta})$. Its algebraic conjugate θ_2 is also in the support of u, and if no other eigenvalue is there, then we are done. Let θ_i be an eigenvalue in the support of u. Then again we can argue that

$$\frac{\theta_1 - \theta_i}{\theta_1 - \theta_2} \in \mathbb{Q}.$$

Note that $(\theta_1 - \theta_2)$ is an integer multiple of $\sqrt{\Delta}$. It follows that $\theta_1 - \theta_i$ is an integer multiple of $\sqrt{\Delta}$ for all θ_i in the eigenvalue support of u. This implies item (ii). $\square$

We will now summarize the work in this section to provide explicit necessary and sufficient conditions for perfect state transfer, this time in the context of graphs. We note that some of the results of the following theorem have been shown in previous works. However, the form presented below is due to the author.

2.4.4 Theorem. *Let X be a graph, $u, v \in V(X)$. Let $\theta_0 > ... > \theta_k$ be the eigenvalues in Φ_u. Then X admits perfect state transfer between u and v if and only if all of the following conditions hold.*

(i) Vertices u and v are strongly cospectral.

(ii) Non-zero elements in Φ_u are either all integers or all quadratic integers. Moreover, there is a square-free integer Δ, an integer a, and integers $b_0, ..., b_k$ such that

$$\theta_r = \frac{1}{2}\left(a + b_r\sqrt{\Delta}\right) \quad \textit{for all } r = 0, ..., k.$$

Here we allow $\Delta = 1$ for the case where all eigenvalues are integers, and $a = 0$ for the case where they are all multiples of $\sqrt{\Delta}$.

(iii) Let $g = \gcd\left(\left\{\frac{\theta_0 - \theta_r}{\sqrt{\Delta}}\right\}_{r=0}^{k}\right)$. Then

a) $\theta_r \in \Phi_{uv}^{+}$ if and only if $\frac{\theta_0 - \theta_r}{g\sqrt{\Delta}}$ is even, and

b) $\theta_r \in \Phi_{uv}^{-}$ if and only if $\frac{\theta_0 - \theta_r}{g\sqrt{\Delta}}$ is odd.

Moreover, if these conditions hold and perfect state transfer occurs between u and v at time τ with phase λ, then *a) There is a minimum time $\tau_0 > 0$ at which perfect state transfer occurs between u and v, and*

$$\tau_0 = \frac{1}{g}\frac{\pi}{\sqrt{\Delta}}.$$

b) The time τ is an odd multiple of τ_0.

c) The phase λ is equal to $\mathtt{e}^{\mathtt{i}\tau\theta_0}$.

Proof. Theorems 2.4.2 and 2.4.3 show that conditions (i) and (ii) are necessary. We assume they are true, and we will show that conditions 2.4.2.b and 2.4.2.c are equivalent to (iii).

Write $\tau = \mu\dfrac{\pi}{\sqrt{\Delta}}$, where $\mu \in \mathbb{R}^+$ is chosen appropriately. From (ii) above, it follows that

$$\frac{\theta_0 - \theta_r}{\sqrt{\Delta}} \in \mathbb{Z}.$$

Conditions 2.4.2.b and 2.4.2.c imply that $\mu = \frac{p}{q}$, with $p, q \in \mathbb{Z}^+$ coprime and p odd. They also imply that for all $\theta_r \in \Phi_u$, the number q divides

$$\frac{\theta_0 - \theta_r}{\sqrt{\Delta}}. \tag{2.15}$$

If this happens, the conditions 2.4.2.b and 2.4.2.c are equivalent to

$$\begin{aligned} \left|\frac{\theta_0 - \theta_r}{\sqrt{\Delta}}\right|_2 &< |q|_2 \quad \text{whenever } \theta_r \in \Phi_{uv}^+, \quad \text{and} \\ \left|\frac{\theta_0 - \theta_r}{\sqrt{\Delta}}\right|_2 &= |q|_2 \quad \text{whenever } \theta_r \in \Phi_{uv}^-. \end{aligned} \tag{2.16}$$

An integer $q \in \mathbb{Z}$ satisfying these properties exists if and only if the largest integer satisfying the properties is the gcd g of the differences as r ranges over $\{1, ..., k\}$.

Now to see a), note that (iii) does not depend on p, so it can chosen to be any odd integer. Because $q \leq g$, it follows that a minimum time exists when $p = 1$ and $q = g$. Property b) follows easily, and c) is in Theorem 2.4.2. $\square$

The following corollary is due to Kay [51], and our proof based on the result above is different than the original.

2.4.5 Corollary. *If perfect state transfer happens in X between u and v, and between u and w, then $v = w$.*

Proof. From Theorem 2.4.4, the minimum time in which perfect state transfer between u and any vertex happens depends uniquely on Φ_u. If τ is such a time, we have

$$U(\tau)\mathbf{e}_u = \lambda_1 \mathbf{e}_v \quad \text{and} \quad U(\tau)\mathbf{e}_u = \lambda_2 \mathbf{e}_w,$$

hence $\mathbf{e}_v = \mathbf{e}_w$. □

2.5 Strong cospectrality

In this section, we examine in more detail what it means for two vertices to be strongly cospectral. We begin with some definitions. Let X be a graph and A its adjacency matrix with spectral decomposition

$$A = \sum_{r=0}^{d} \theta_r E_r.$$

Definition. We say that $u, v \in V(X)$ are *cospectral* if the spectra of the graphs $X \backslash u$ and $X \backslash v$ are equal.

Definition. We say that $u, v \in V(X)$ are *parallel* if $E_r \mathbf{e}_u$ is a multiple of $E_r \mathbf{e}_v$ for all $r \in \{0, ..., d\}$ whenever $E_r \mathbf{e}_v \neq \mathbf{0}$.

Definition. The *walk generating function* of a graph X on n vertices is

$$W(X, t) = \sum_{k \geq 0} t^k A^k \tag{2.17}$$

and the *walk matrix* of a subset $S \subset V(X)$ with characteristic vector $\mathbf{w} = \mathbf{w}_S$ is

$$M_S = \left(\begin{array}{c|c|c|c} \mathbf{w} & A\mathbf{w} & \cdots & A^{n-1}\mathbf{w} \end{array} \right) \tag{2.18}$$

We will see that two vertices are strongly cospectral if and only if they are cospectral and parallel, but first we present a characterization of cospectral vertices due partly to Godsil and McKay (see [38]) and partly to Godsil. The corollary is due to Godsil (unpublished notes).

2.5.1 Theorem. *Let $u, v \in V(X)$. The following statements are equivalent.*

(i) u and v are cospectral.

(ii) $W(X,t)_{u,u} = W(X,t)_{v,v}$.

(iii) For each E_r, with $r = 0, ..., d$, we have $(E_r)_{u,u} = (E_r)_{v,v}$.

(iv) With $M_{\{u\}} = M_u$, we have $M_u^T M_u = M_v^T M_v$.

(v) The subspace $\langle\{A^k(\boldsymbol{e}_u + \boldsymbol{e}_v)\}_{k\geq 0}\rangle$ is orthogonal to the subspace $\langle\{A^k(\boldsymbol{e}_u - \boldsymbol{e}_v)\}_{k\geq 0}\rangle$.

(vi) There is an orthogonal matrix Q that commutes with A such that $Q^2 = I$ and $Q\boldsymbol{e}_u = \boldsymbol{e}_v$.

Proof.

(i) ⇔ (ii) Note that

$$W(X,t) = (\mathtt{I} - tA)^{-1} = t^{-1}(t^{-1}\mathtt{I} - A)^{-1}.$$

Let $\phi_X(t)$ denote the characteristic polynomial of $A(X)$ with variable t. From Gabriel's rule[1], for all $w \in V(X)$,

$$[(s\mathtt{I} - A)^{-1}]_{w,w} = \frac{\det(s\mathtt{I} - A(X\backslash w))}{\det(s\mathtt{I} - A(X))} = \frac{\phi_{X\backslash w}(s)}{\phi_X(s)},$$

So $W(X,t)_{u,u} = W(X,t)_{v,v}$ if and only if $\phi_{X\backslash u}(t) = \phi_{X\backslash v}(t)$.

(ii) ⇔ (iii) From Equation 2.17, (ii) holds if and only if $(A^k)_{u,u} = (A^k)_{v,v}$ for all $k \geq 0$. From Corollary 2.1.7, this is equivalent to $(E_r)_{u,u} = (E_r)_{v,v}$ for all $r = 0, ..., d$.

[1]See Gabriel Cramer [23].

(ii) $\Leftrightarrow$ (iv) Note that for any $w \in V(X)$, we have $(M_w^T M_w)_{ij} = \mathbf{e}_w^T A^{i+j-2} \mathbf{e}_w$, so (ii) is equivalent to (iv).

(iii) $\Leftrightarrow$ (v) From Corollary 2.1.7, for all r and s, (v) is equivalent to

$$(\mathbf{e}_u + \mathbf{e}_v)^T E_r^T E_s (\mathbf{e}_u - \mathbf{e}_v) = \mathbf{0}.$$

This is trivially true if $r \neq s$ because then $E_r E_s = \mathtt{0}$. If $r = s$, then

$$(\mathbf{e}_u + \mathbf{e}_v)^T E_r^T E_r (\mathbf{e}_u - \mathbf{e}_v) = \mathbf{e}_u^T E_r \mathbf{e}_u - \mathbf{e}_v^T E_r \mathbf{e}_v,$$

which is $\mathbf{0}$ if and only if (iii) holds.

(v) $\Rightarrow$ (vi) Any linear transformation is defined in terms of its action on a subspace S and its orthogonal complement $S^\perp$. Let $S = \langle \{A^k(\mathbf{e}_u - \mathbf{e}_v)\}_{k \geq 0} \rangle$. Define a matrix Q by

$$Q\mathbf{v} = \begin{cases} -\mathbf{v} & \text{if } \mathbf{v} \in S, \\ \mathbf{v} & \text{if } \mathbf{v} \in S^\perp. \end{cases}$$

Note that Q is orthogonally diagonalizable, hence symmetric, and that $Q^2 = \mathtt{I}$, thus Q is an orthogonal matrix. Now Q commutes with A both in S and in $S^\perp$, so it commutes with A in general, and finally, from (v), Q fixes $\langle \{A^k(\mathbf{e}_u + \mathbf{e}_v)\}_{k \geq 0} \rangle$. Hence

$$2Q\mathbf{e}_u = Q[(\mathbf{e}_u + \mathbf{e}_v) + (\mathbf{e}_u - \mathbf{e}_v)] = (\mathbf{e}_u + \mathbf{e}_v) + (\mathbf{e}_v - \mathbf{e}_u) = 2\mathbf{e}_v.$$

(vi) $\Rightarrow$ (iii) Let Q satisfy (vi). Then for all $r = 0, ..., d$, Corollary 2.1.7 implies that Q commutes with E_r, hence

$$\mathbf{e}_u^T E_r \mathbf{e}_u = \mathbf{e}_u^T E_r Q^2 \mathbf{e}_u = \mathbf{e}_u^T Q^T E_r Q \mathbf{e}_u = \mathbf{e}_v^T E_r \mathbf{e}_v.$$

□

2.5.2 Corollary. *Vertices u and v are strongly cospectral if and only if they are cospectral and parallel.*

Proof. Clearly if u and v are strongly cospectral, then they are parallel. So we suppose they are parallel and show that strong cospectrality is equivalent to cospectrality. First note that $\langle E_r\mathbf{e}_u, E_r\mathbf{e}_v\rangle = (E_r)_{u,u}$, thus $E_r\mathbf{e}_u = \mathbf{0}$ if and only if $(E_r)_{u,u} = 0$. So if u and v are cospectral or if u and v are strongly cospectral, it follows that $E_r\mathbf{e}_u = \mathbf{0}$ if and only if $E_r\mathbf{e}_v = \mathbf{0}$ for all r.

Now suppose that $E_r\mathbf{e}_u = \lambda E_r\mathbf{e}_v \neq \mathbf{0}$. Then

$$(E_r)_{u,u} = \lambda(E_r)_{u,v} = \lambda(E_r)_{v,u} = \lambda^2(E_r)_{v,v},$$

thus they are strongly cospectral if and only if they are cospectral. $\square$

2.5.3 Corollary. *The vertices u and v are strongly cospectral if and only if there is a matrix Q satisfying the following conditions.*

(i) Q is orthogonal, commutes with A, and satisfies $Q^2 = I$ and $Q\boldsymbol{e}_u = \boldsymbol{e}_v$.

(ii) Q is a polynomial in A.

Proof. We use the same construction as in Theorem 2.5.1, and so we just need to prove the equivalence with (ii). If u and v are strongly cospectral, then the invariant subspaces of Q are spanned by eigenvalues of A, hence if $p(x)$ is a polynomial such that

$$p(\theta_r) = \begin{cases} -1 & \text{if } \theta_r \in \Phi_{uv}^-, \\ 1 & \text{otherwise,} \end{cases}$$

then $p(A) = Q$. If Q is a polynomial in A, then it must be a signed sum of the idempotents of A, and hence $Q\mathbf{e}_u = \mathbf{e}_v$ implies $E_r\mathbf{e}_u = \pm E_r\mathbf{e}_v$ for all r. $\square$

Chapter 3

Distance-regular graphs and association schemes

This chapter includes part of the material presented in Coutinho et al [21]. In Section 3.1, we develop a self contained introduction to distance-regular graphs and association schemes. In the remaining sections, we will focus on the problem of finding new examples of perfect state transfer. In Section 3.2, we present a necessary and sufficient condition for a distance-regular graph to admit perfect state transfer, and as a consequence we find all known distance-regular graphs that do so. Section 3.3 contains some results relating perfect state transfer and graphs whose adjacency matrix belongs to the Bose-Mesner Algebra of an association scheme.

3.1 Preliminaries

The classical reference for the study of distance-regular graphs is Brouwer, Cohen and Neumaier (BCN) [13].

Definition. A set $\{A_0, ..., A_d\}$ of 01-matrices of size $n \times n$ is a (symmetric) *association scheme* if the following properties hold:

(i) the identity matrix $\mathtt{I}$ belongs to the set, say $A_0 = \mathtt{I}$;

(ii) A_i is symmetric for $i = 0, \dots, d$;

(iii) $\displaystyle\sum_{k=0}^{d} A_k = \mathtt{J}$; and,

(iv) there exist integers p_{ij}^k, called *intersection numbers of the scheme* , such that:

$$A_i A_j = \sum_{k=0}^{d} p_{ij}^k A_k.$$

Definition. The matrices in $\{A_0, ..., A_d\}$ are called the *classes* of the scheme. The matrix algebra spanned by these matrices is the *Bose-Mesner algebra* of scheme, and is usually denoted by the symbol $\mathcal{A}$.

We will say that a graph *belongs to an association scheme* if its adjacency matrix is contained in the Bose-Mesner algebra of the scheme.

Note that (ii) and (iv) imply that $A_0, ..., A_d$ pairwise commute. Hence $\mathcal{A}$ is a commutative algebra, and the fact that $\mathtt{J}$ belongs to the algebra implies that any matrix in the algebra has constant row and column sums.

Definition. The *Schur product* of matrices M and N of the same size is defined as

$$(M \circ N)_{a,b} = M_{a,b} \cdot N_{a,b}.$$

Note that for an association scheme $\{A_0, ..., A_d\}$, property 3.1.(iii) implies that

$$A_i \circ A_j = \begin{cases} A_i & \text{if } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Thus the Bose-Mesner algebra is closed under Schur product, and the matrices $\{A_0, ..., A_d\}$ are idempotents with respect to this product, also called *Schur idempotents*. A set of symmetric and pairwise commuting matrices can be simultaneously diagonalized (see Theorem

2.1.8), hence there exist idempotents for the conventional matrix product $\{E_0, ..., E_m\}$ which also form a basis for the Bose-Mesner algebra. In particular $m = d$ and any matrix in $\mathcal{A}$ has at most $d+1$ distinct eigenvalues.

The construction of non-trivial association schemes is not an easy task. We now describe a construction based on graphs that exhibit a high level of regularity.

Definition. A connected graph X of diameter d is called a *distance-regular graph* if there exist numbers $b_i,\ c_i$ with $0 \leq i \leq d$ such that for any two vertices u and v at distance i in X, the number of neighbours of v at distance $i-1$ from u is c_i and the number of neighbours of v at distance $i+1$ from u is b_i (note that these numbers do not depend on the choice of u and v). Here we convention that $c_{-1} = 0$.

This definition implies that the graph is regular with valency b_0, and also that there exist numbers a_i which are the number of neighbours of v at distance i from u. They do not depend on u and v because a_i is determined in terms of b_i and c_i by

$$b_0 = c_i + a_i + b_i. \tag{3.1}$$

Definition. Let X be a distance-regular graph of diameter d. The *intersection array* of X is the list of parameters $\{b_0, b_1, ..., b_{d-1};\ c_1, c_2, ..., c_d\}$.

The following proposition provides a well-known necessary condition for an array of numbers to be the intersection array of a distance-regular graph.

3.1.1 Proposition (BCN [13], Proposition 4.1.6)**.** *If $\{b_0, b_1, ..., b_{d-1};\ c_1, c_2, ..., c_d\}$ is the intersection array of a distance-regular graph, then $b_0 > b_1 \geq b_2 \geq ... \geq b_{d-1} > 0$ and $1 = c_1 \leq c_2 \leq ... \leq c_d \leq b_0$.*

Definition. Given X, we define the *distance graphs* X_i as the graphs with vertex set $V(X)$ and two vertices adjacent if and only if they are at distance i in X. We also define *distance matrices* $A_i(X) = A(X_i)$, with $A_0 = \mathtt{I}$.

By definition of a distance-regular graph, the matrices $\{A_0,\ A,\ A_2,\ ...,\ A_d\}$ satisfy

$$AA_i = b_{i-1}A_{i-1} + a_iA_i + c_{i+1}A_{i+1}. \tag{3.2}$$

In particular, the matrices A_i can be written as a polynomial of degree i in A for all $i \geq 1$. By induction and using the equation above, one can prove that there exist *intersection numbers of the graph* p_{ij}^k, which depend only on the intersection array, such that

$$A_i A_j = \sum_{k=0}^{d} p_{ij}^k A_k.$$

The combinatorial interpretation of these numbers is that for any two vertices u and v at distance k, there are precisely p_{ij}^k vertices in the graph at distance i from u and j from v.

If X is a distance-regular graph of diameter d, the matrices $\{A_0, A_1, ..., A_d\}$ form an association scheme, and the intersection numbers of the graph coincide with those of the scheme.

Definition. A distance-regular graph X of diameter d is *primitive* if the graphs X_i for $i \in \{1, ..., d\}$ are all connected, and *imprimitive* otherwise.

Definition. If X_d is the disjoint union of cliques of the same size, then X is called *antipodal*, and the cliques in X_d are the *fibres* or antipodal classes of the graph. If a fibre contains only two vertices, we will say that they are antipodal vertices of the graph.

3.1.2 Theorem (BCN [13], Theorem 4.2.1)**.** *Let X be a distance-regular graph of valency at least* 3*. If X is imprimitive, then X is either bipartite or antipodal.*

We end this section with a remark about distance-regular graphs and association schemes. Typically, one wishes to find new constructions of such structures, or to find constraints that the intersection numbers must satisfy. Intersection numbers that correspond to known constructions or that cannot be ruled out by any known constraints are usually called *feasible parameter sets*. Despite the efforts of many in the past decades, the gap between the known constructions and the feasible parameter sets is still very large. No original work in this thesis succeeds in reducing this gap[1]. We will rather examine feasible parameter sets and determine whether or not a corresponding graph admits perfect state transfer.

[1]But surely wishes.

3.2 Perfect state transfer on distance-regular graphs

We start this section with a necessary condition for graphs belonging to association schemes to admit perfect state transfer. The result is due to Godsil [33], and the explicit proof below is from Coutinho et al. [21].

3.2.1 Theorem ([33], Theorem 4.1 and Lemma 6.1)**.** *Let X be a graph that belongs to an association scheme with $d+1$ classes and with adjacency matrix A. If X admits perfect state transfer at time τ, then there is a permutation matrix T with no fixed points and of order two such that $U_A(\tau) = \lambda T$ for some $\lambda \in \mathbb{C}$. Moreover, T is a class of the scheme. If the graph is distance-regular of diameter d, then it must be antipodal with fibres of size 2 and $T = A_d$.*

Proof. Recall from Equation 2.11 that $U(t) = \sum_{r=0}^{d} \mathrm{e}^{\mathrm{i}t\theta_r} E_r$. Thus, for any $t \in \mathbb{R}$, the matrix $U(t)$ belongs to the Bose-Mesner algebra of the scheme. Let $u, v \in V(X)$ be such that $U(\tau)\mathbf{e}_u = \lambda \mathbf{e}_v$. Any matrix in the algebra commutes with $\mathtt{J}$ and so has constant row and column sums. The matrix $U(\tau)$ has a row with a unique non-zero entry and it can be written as a linear combination of Schur idempotents. Because the Schur idempotents have disjoint support, $U(t)$ must be a multiple of one Schur idempotent T.

Note that $T\mathbf{e}_u = \mathbf{e}_v$. So the row and column sums of T are equal to 1. Therefore T is a permutation matrix. Since $T \neq A_0$, the permutation represented by T has no fixed points, and because $U(\tau)$ is symmetric, we have that T is a permutation matrix of order 2.

Now if X is distance-regular, let i be the index for which $A_i = T$. Suppose $0 < i < d$, and so $d > 1$. Because v is the only vertex at distance i from u, we have $b_{i-1} = 1$. By Proposition 3.1.1, this implies that $b_j = 1$ for all $j \geq i$. In particular, there will be a unique vertex at distance d from u, and this vertex will have degree 1, so $b_0 = 1$ and therefore the graph is K_2 and $d = 1$, a contradiction. Therefore $A_d = T$, and the distance-regular graph is antipodal with fibres of size 2. □

In the context of Theorem 3.2.1, perfect state transfer in a distance-regular graph must be between a pair of antipodal vertices.

3.2.2 Lemma. *If X is an antipodal distance-regular graph with fibres of size 2, distinct eigenvalues $\theta_0 > \ldots > \theta_d$, and if u and v are a pair of antipodal vertices, then*

(i) u and v are strongly cospectral, and

(ii) $E_r \boldsymbol{e}_u = (-1)^r E_r \boldsymbol{e}_v$ for all idempotents E_r, with $r = 0, \ldots, d$.

Proof. Note that (ii) $\implies$ (i) trivially. Condition (ii) is simply a consequence of known results about sign changes in Sturm sequences (see Godsil [36, Section 8.5]), but we will provide an elementary proof of this fact in Chapter 6. $\square$

If X is a distance-regular graph, note that the idempotents E_r are linear combinations of the distance matrices of X. Thus each row or column of each E_r contains non-zero elements. As a consequence, the eigenvalue support of each vertex in a distance-regular graph is equal to the set of all distinct eigenvalues of X.

We present the following characterization of perfect state transfer in distance-regular graphs.

3.2.3 Theorem. *Suppose X is a distance-regular graph with distinct eigenvalues $\theta_0 > \ldots > \theta_d$. Then X admits perfect state transfer between vertices u and v at time τ if and only the following holds.*

(i) The eigenvalues of X are integers.

(ii) X is antipodal with fibres of size 2, and u and v are antipodal vertices.

(iii) If $g = \gcd(\{\theta_0 - \theta_r\}_{r=1}^{d})$, then

a) $\dfrac{\theta_0 - \theta_r}{g}$ is even for all r even.

b) $\dfrac{\theta_0 - \theta_r}{g}$ is odd for all r odd.

Under these condition, $\tau_0 = \dfrac{\pi}{g}$ is the minimum time at which perfect state transfer between u and v occurs.

Proof. Because X is regular, Corollary 2.1.10 implies that there is at least one non-zero integer in the eigenvalue support of each vertex of X. Thus Theorem 2.4.3 implies that (i) is a necessary condition. From Theorem 3.2.1, (ii) is necessary. Now suppose both are true.

In the context of Theorem 2.4.4, Lemma 3.2.2 is saying that $\theta_r \in \Phi^+_{uv}$ if r is even, and $r \in \Phi^-_{uv}$ if r is odd. Thus condition (iii) above is equivalent to condition 2.4.4.(iii), and so equivalent to the existence of perfect state transfer between u and v. The expression for the time also follows from Theorem 2.4.4. □

We have an important remark at this point. The distance partition relative to a fixed vertex in any distance-regular graph is an *equitable partition*. Its quotient is a weighted path with loops allowed at each vertex. A consequence of Theorem 3.2.1 is that if a distance-regular graph X admits perfect state transfer between u and v, then $\{u\}$ and $\{v\}$ are singletons at maximum distance in the distance partition of u. It follows that perfect state transfer also happens between these two vertices in the corresponding weighted path, and that any simple graph in which the quotient of the distance partition relative to u is equal to that weighted path will also admit perfect state transfer between u and v. In other words, we can alter the edges in X maintaining the parameters of the distance partition of u and still have perfect state transfer. The downside is that this new graph will most likely no longer be a distance-regular graph, and so perfect state transfer will happen between u and v, but usually not between any other pair of vertices. In our approach below, we will focus only on finding distance-regular graphs admitting perfect state transfer, even though we could find many more examples based on each of them.

Quotienting and lifting in the context of perfect state transfer was studied in [5]. We will readdress this topic in Chapter 6, including a better explanation of the discussion above. For now, we determine which known distance-regular graphs admit perfect state transfer.

3.2.1 Diameter two

The observation in this subsection is due to Coutinho et al. [21].

The distance-regular graphs of diameter 2 are also known as *(connected) strongly regular graphs* (see Godsil and Royle [42, Chapter 10]).

The intersection array of a strongly regular graph is determined by the 4-tuple (n, k, a, c), where n is the number of vertices, k is the valency, a is the number of common neighbours of two adjacent vertices, and c is the number of common neighbours of two non-adjacent vertices. Such a graph is antipodal if and only if being at distance 0 or 2 is an equivalence relation, and in terms of the parameters, this implies that $c = k$ and $a = 2k - v$. It follows that the graphs are complete multipartite with classes of size $v - k$. By Theorem 3.2.1, perfect state transfer happens only if $v - k = 2$, in which case the graph is the complement of a disjoint union of m copies of K_2. The distinct eigenvalues of such graphs are

$$\{2m - 2,\ 0,\ -2\}.$$

Hence, using Theorem 3.2.3, we have:

3.2.4 Corollary. *Perfect state transfer happens in distance-regular graphs of diameter* 2 *if and only if the graph is the complement of a disjoint union of m copies of K_2 with m even. In that case, perfect state transfer happens at time $\frac{\pi}{2}$.*

3.2.2 Diameter three

Antipodal distance-regular graphs of diameter 3 have a special structure that we introduce below.

Definition. A graph X is called a *covering graph* if there is a partition of its vertex set into independent cells such that between any two such cells either there are no edges or there is a perfect matching. We say that X is a covering of Y if the vertices of Y correspond to the cells of the partition on X, two vertices of Y being adjacent if and only if there is a matching between the corresponding cells. If Y is connected, all cells of X must have the same size, say r, and in this case X is an *r-fold covering* of Y.

We refer to Sections 2 and 3 of Godsil and Hensel [37] for the basic results about antipodal distance-regular graphs of diameter three that we present below.

3.2.5 Theorem ([37], Theorem 2.1)**.** *Any antipodal distance-regular graph of diameter 3 is an r-fold covering of K_n for some n. The size of each antipodal class is equal to r.*

Recall from Section 3.1 the definition of intersection numbers and intersection array of a distance-regular graph.

3.2.6 Theorem ([37], Lemma 3.1)**.** *Let X be a distance-regular r-fold covering of K_n. Let $c = p^2_{11}$, that is, the number of common neighbours of two vertices at distance 2. Then the intersection numbers of X depend only on n, r and c, and the intersection array of X is given by*

$$\{n-1,\ (r-1)c,\ 1;\ 1,\ c,\ n-1\}$$

Definition. We will refer to antipodal distance-regular graphs of diameter 3 with parameters (n, r, c) as (n, r, c)*-covers*. Given a (n, r, c)-cover, we define the parameters

$$\delta = n - rc - 2 \quad \text{and} \quad \Delta = \delta^2 + 4(n-1).$$

3.2.7 Theorem ([37], Section 3)**.** *The distinct eigenvalues of a (n, r, c)-cover are*

$$\left\{n-1,\ \frac{\delta+\sqrt{\Delta}}{2},\ -1,\ \frac{\delta-\sqrt{\Delta}}{2}\right\}. \tag{3.3}$$

And finally, a theorem due to Godsil and Hensel.

3.2.8 Theorem ([37], Theorem 3.6)**.** *For fixed values of r and δ, there are only finitely many feasible parameter sets for distance-regular covers of K_n, unless $\delta = -2$, $\delta = 0$ or $\delta = 2$.*

Recall that r is the size of an antipodal class. By Theorem 3.2.1, a search for perfect state transfer in (n, r, c)-covers only needs to consider the case where $r = 2$. We assume $r = 2$ henceforth.

3.2.9 Theorem ([42], Chapter 11)**.** *Let X be a $(n, 2, c)$-cover. The graph induced by the neighbourhood of a vertex of X is a strongly regular graph with parameters*

$$\left(n-1,\ n-c-2,\ n-\frac{3c}{2}-3,\ \frac{n-c-2}{2}\right).$$

Equivalently, any strongly regular graph with such parameters can be extended to construct a $(n, 2, c)$*-cover.*

We now start our classification of $(n, 2, c)$-covers admitting perfect state transfer. We proceed via the case analysis suggested by Theorem 3.2.8.

3.2.10 Theorem. *A* $(n, 2, c)$*-cover with* $\delta = 0$ *does not admit perfect state transfer.*

Proof. If $\delta = 0$, then $n = 2c + 2$ and $\Delta = 4(n - 1)$, and the distinct eigenvalues are

$$\{n - 1,\ \sqrt{n-1},\ -1,\ -\sqrt{n-1}\}.$$

If perfect state transfer occurs, Theorem 3.2.3 implies that the eigenvalues must be integers, hence $(n - 1)$ must be a square, thus n is congruent to 2 modulo 4. Note that $n = (n - 1) - (-1)$ and $(n - 1)$ and (-1) are eigenvalues with the same parity. Therefore Theorem 3.2.3 implies that if perfect state transfer occurs in this case, it will occur at time $\frac{\pi}{b}$, with b an odd number, and so the differences between eigenvalues with different parities must be odd. But $\sqrt{n-1}$ and $n - 1$ are both odd, hence their difference is even. We conclude that in this case perfect state transfer cannot occur. □

For $\delta \neq 0$, the following proposition says that the other cases occur in pairs (see for instance BCN [13, p.431]).

3.2.11 Proposition. *Suppose* X *is* $(n, 2, c)$*-cover. Then the distance 2 graph* X_2 *is a* $\big(n, 2, (n - c - 2)\big)$*-cover, and so* $\delta(X_2) = -\delta(X)$*.*

We determine the structure of the $(n, 2, c)$-covers with $\delta = -2$. We will provide a simplified form of [37, Lemma 8.2] and a proof due to the author, but first a definition.

Definition. A *Hadamard matrix* of order n is a $n \times n$ matrix H with entries in $\{1, -1\}$ such that

$$HH^T = H^T H = I_n.$$

Example 4. The following matrix is an example of a symmetric Hadamard matrix with constant diagonal,

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix},$$

and so by Theorem 3.2.12 below is equivalent to a $(4, 2, 2)$-cover. In this case, the graph will be the cube.

Let X be a $(n, 2, c)$-cover with $\delta = -2$. Order the antipodal pairs from 1 to n, and for each antipodal pair define an arbitrary ordering of its vertices. Define a square matrix B of order n indexed by the antipodal pairs of X as follows.

$$B_{ij} = \begin{cases} 0, & \text{if } i = j; \\ +1, & \text{if the matching between pairs } i \text{ and } j \text{ agrees with their} \\ & \text{respective orderings;} \\ -1, & \text{otherwise.} \end{cases}$$

3.2.12 Theorem. *Given a $(n, 2, c)$-cover with $\delta = -2$ and a matrix B as above, the matrix $(B+I)$ is a symmetric Hadamard matrix with constant diagonal. Conversely, every symmetric Hadamard matrix with constant diagonal and order n yields a $\left(n, 2, \frac{n}{2}\right)$-cover.*

Proof. Clearly the diagonal entries of $(B+I)^2$ are equal to n. Now consider an entry (i, j), associated to antipodal pairs (a_i, b_i) and (a_j, b_j). If $a_i \sim a_j$ and $b_i \sim b_j$, then $(B+I)_{ij} = 1$. Whenever rows i and j agree in a coordinate k which is neither i or j, that means we have a common neighbour of a_i and a_j, and if they disagree, we have a common neighbour of a_i and b_j. Hence they agree in $(n - c - 2)$ coordinates and disagree in c of them. So the dot product of rows i and j is equal to $2+(n-c-2)-c = 0$ if and only if $\delta = -2$. If $a_i \sim b_j$ and $a_j \sim b_i$, we have that the dot product between rows i and j will be $-2-(n-c-2)+c = 0$ again. So $(B + I)$ is a symmetric Hadamard matrix of constant diagonal. The converse is proved similarly. $\square$

Example 5. Consider the Hadamard matrix of Example 4. Following the steps of the proof above, we can easily construct the adjacency matrix of the corresponding $(4, 2, 2)$-cover as follows. First turn the diagonal entries into 0. Replace these entries by the zero matrix of dimension two, then replace all entries equal to $+1$ by $\mathtt{I}_2$, and all entries equal to -1 by $A(K_2)$. The resulting matrix is the adjacency matrix of the cube:

$$\begin{pmatrix} 0 & 0 & 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 & 1 & 0 & 0 & 0 \end{pmatrix}.$$

If X is a $(n, 2, c)$-cover with $\delta = -2$, it follows from arithmetic conditions on the multiplicities of the eigenvalues of X that n must be a square (see Godsil and Hensel [37, Lemma 3.7]). This can also be derived as a necessary condition for the existence of symmetric Hadamard matrices of constant diagonal.

It is also a known fact that Hadamard matrices can only exist when n is 1, 2 or a multiple of 4 (see for instance BCN [13, Section 1.8]).

3.2.13 Theorem. *Every $(n, 2, c)$-cover with $\delta = -2$ admits perfect state transfer at time $\frac{\pi}{\sqrt{n}}$. For $\delta = +2$, perfect state transfer occurs if and only if n is divisible by 8, and in that case it occurs at time $\frac{\pi}{2}$.*

Proof. Let X be a $(n, 2, c)$-cover with $\delta = -2$, and so n is an even perfect square. Using Equation 3.3, its set of distinct eigenvalues will be

$$\{n - 1,\ \sqrt{n} - 1,\ -1,\ -\sqrt{n} - 1\}.$$

Applying Theorem 3.2.3, we see that perfect state transfer will occur at time $\dfrac{\pi}{\sqrt{n}}$. If $\delta = +2$, then the set of distinct eigenvalues is

$$\{n - 1,\ \sqrt{n} + 1,\ -1,\ -\sqrt{n} + 1\}.$$

If $|n|_2 = 2^{-2}$, then $|(n-1) - (\sqrt{n}+1)|_2 = |(n-1) - (-1)|_2$, and so perfect state transfer cannot occur. If $|n|_2 < 2^{-2}$, then it is easy to check that perfect state transfer will occur at time $\frac{\pi}{2}$. □

Symmetric Hadamard matrices of order n with constant diagonal can be constructed for every n which is a power of 4 as the iterated Kronecker product of the matrix depicted in Example 4.

Perfect state transfer was already known for the case $\delta = -2$ (see Godsil [33]), but unknown for the case $\delta = +2$.

Now we move to the case where $\delta \notin \{0, -2, 2\}$. As we saw in Proposition 3.2.11, for every cover with parameter δ, there exists a corresponding cover with parameter $-\delta$.

3.2.14 Theorem. *Let X be a $(n, 2, c)$-cover, and X_2 the corresponding $(n, 2, n-c-2)$-cover. Suppose $\delta \notin \{0, -2, 2\}$.*

a) If $\delta \equiv 2 \bmod 4$, then perfect state transfer occurs either in X or in X_2 at time $\frac{\pi}{2\alpha}$, for some α which is an odd integer.

b) If δ is odd or a multiple of 4, perfect state transfer does not occur in either X or X_2.

Proof. Let $\rho > 0$ and $\sigma < 0$ be the eigenvalues of X which are neither $(n-1)$ nor -1. Let m_ρ and m_σ be their corresponding multiplicities, which can be computed in terms of n, r and c (see Godsil and Hensel [37, Section 3]). Then

$$m_\rho - m_\sigma = \frac{n\delta}{\sqrt{\Delta}},$$

This is a difference of integers, so $\delta \neq 0$ implies that Δ must be a perfect square. Note that $\sigma = \frac{1}{2}(\delta - \sqrt{\Delta})$ is an algebraic integer, hence an integer. Thus $\sqrt{\Delta} - \delta$ is even. Suppose that $\Delta = (2t + \delta)^2$. The parameter n is now parametrized as $n = 1 + t^2 + t\delta$.

Note that if n is odd, then perfect state transfer cannot occur by Theorem 3.2.3. If δ is odd, then $n = \delta + 2c + 2$ is odd. If t is even, then n is also odd. So suppose δ is even and t is odd.

If δ is a multiple of 4, then $n = 1 + t^2 + t\delta \equiv 2 \bmod 4$. Perfect state transfer occurs only if $(n-1) - \rho$ and $(n-1) - \sigma$ are both odd. Hence ρ and σ are both even. But note that $\sigma = -t$ and t is odd.

If $\delta \equiv 2 \bmod 4$, then $n = 1 + t^2 + t\delta \equiv 0 \bmod 4$. Let $\rho_2 > 0$ and $\sigma_2 > 0$ be the non-trivial eigenvalues of X_2. Note that:

$$\rho = \delta + t \quad \text{and} \quad \sigma = -t,$$

and

$$\rho_2 = t \quad \text{and} \quad \sigma_2 = -\delta - t.$$

If $t \equiv 3 \bmod 4$, then $(n-1) - (\delta + t)$ and $(n-1) + t$ are both congruent to 2 modulo 4, so by Theorem 3.2.3 perfect state transfer occurs in X at time $\frac{\pi}{2\alpha}$, where 2α is the greatest common divisor of the differences of the eigenvalues of X. If $t \equiv 1 \bmod 4$, then $(n-1) - t$ and $(n-1) - (-\delta - t)$ are both congruent to 2 modulo 4, so perfect state transfer occurs in X_2 at time $\frac{\pi}{2\alpha}$, where 2α is the greatest common divisor of the differences of the eigenvalues of X_2. $\square$

Note that in the case where $\delta \equiv 2 \bmod 4$, the theorem above implies that perfect state transfer occurs in at least one of X and X_2. It is possible that perfect state transfer occurs in both, but in that case it will be at different times.

Table 3.1 below contains parameter sets for which a corresponding cover admits perfect state transfer, for $n < 280$. The strongly regular graph on the first neighbourhood of a vertex in each of these covers is given in the rightmost column. We consult Andries Brouwer's website (http://www.win.tue.nl/∼aeb/graphs/srg/srgtab.html) to either provide a construction for such a graph, hence a construction for the cover, or to state that no such construction is known.

Table 3.1: Perfect state transfer in distance-regular graphs of diameter 3.

n	c	δ	time	construction of strongly regular graph
28	10	6	$\pi/2$	complement of Schläfli graph
76	42	-10	$\pi/2$	not known
96	40	14	$\pi/4$	not known
96	54	-14	$\pi/6$	not known
120	54	10	$\pi/6$	complement of $O^{-}(8,2)$ polar graph
136	70	-6	$\pi/2$	complement of $O^{+}(8,2)$ polar graph
148	66	14	$\pi/2$	not known
176	72	30	$\pi/4$	complement of the one below
176	102	-30	$\pi/2$	line graph of Hoffman-Singleton graph
244	130	-18	$\pi/2$	not known
276	162	-50	$\pi/6$	complement of McLaughlin graph McL.2 / U4(3).2

3.2.3 Larger diameter

We do not analyse this case in the same detail as we did for the diameter three case. The reason is that the known constructions of antipodal distance-regular graphs of diameter > 3 are scarcer, and so we prefer to just exhibit which known graphs admit perfect state transfer. The work in this subsection is due to Coutinho et al. [21].

The results below are straightforward corollaries of Theorem 3.2.3. We refer to BCN [13, Chapters 9, 11 and 13] for the definition and further details of the graphs mentioned in them.

3.2.15 Corollary. *The graphs below are examples of distance-regular graphs of diameter larger than three admitting perfect state transfer.*

(i) Hamming d-cubes. Number of vertices: 2^d. Valency: d. Diameter: d. Distinct eigenvalues: $\{d-2i : i = 0, ..., d\}$. Time of perfect state transfer: $\frac{\pi}{2}$.

(ii) *Halved 2d-cubes. Number of vertices:* 2^{2d-1}. *Valency:* $\binom{2d}{2}$. *Diameter:* d. *Distinct eigenvalues:* $\left\{\binom{2d}{2} - 2i(2d-i) : i = 0, ..., d\right\}$. *Time of perfect state transfer:* $\frac{\pi}{2}$.

(iii) *Hadamard graphs*[2] *of order* n *if and only if* n *is a perfect square. Exist for infinitely many values of* n*, in particular for all* n *which are powers of* 4. *Number of vertices:* $4n$. *Valency:* n. *Diameter:* 4. *Time of perfect state transfer:* $\frac{\pi}{\sqrt{n}}$.

(iv) *Meixner graph (Martin et al. [58, Example 3.5]). Number of vertices:* 1344. *Valency:* 176. *Diameter:* 4. *Distinct eigenvalues:* $\{176, 44, 8, -4, -16\}$. *Time of perfect state transfer:* $\frac{\pi}{12}$.

(v) *Coset graph of the once shortened and once truncated binary Golay code. Number of vertices:* 1024. *Valency:* 21. *Diameter:* 6. *Distinct eigenvalues:* $\{21, 9, 5, 1, -3, -7, -11\}$. *Time of perfect state transfer:* $\frac{\pi}{4}$.

(vi) *Coset graph of the shortened binary Golay code. Number of vertices:* 2048. *Valency:* 22. *Diameter:* 6. *Distinct eigenvalues:* $\{22, 8, 6, 0, -2, -8, -10\}$. *Time of perfect state transfer:* $\frac{\pi}{2}$.

(vii) *Double coset graph of truncated binary Golay code. Number of vertices:* 2048. *Valency:* 22. *Diameter:* 7. *Distinct eigenvalues:* $\{22, 10, 6, 2, -2, -6, -10, -22\}$. *Time of perfect state transfer:* $\frac{\pi}{4}$.

(viii) *Double coset graph of binary Golay code. Number of vertices:* 4096. *Valency:* 23. *Diameter:* 7. *Distinct eigenvalues:* $\{23, 9, 7, 1, -1, -7, -9, -23\}$. *Time of perfect state transfer:* $\frac{\pi}{2}$.

3.2.16 Corollary. *No graph in the following infinite families of antipodal distance-regular graphs with classes of size two admits perfect state transfer.*

(i) *Johnson graphs* $J(2n, n)$ *for* $n > 1$. *Their distinct eigenvalues are* $\{(n-j)^2 - j\}$*, with* $j \in \{0, ..., n\}$.

(ii) *Doubled odd graphs on* $2n+1$ *points. Their distinct eigenvalues are* $\{(-1)^j(n+1-j)\}$*, with* $j \in \{0, 1, ..., n-1, n, n+2, n+3, ..., 2n+2\}$.

[2] These are not those mentioned in Subsection 3.2.2.

We also checked graphs with diameter larger than 3 depicted in tables of BCN [13, Chapter 14] that do not belong to the infinite families above.

3.2.17 Corollary. *None of the following antipodal distance-regular graphs with classes of size two and diameter larger than three admit perfect state transfer.*

(i) *Wells graph of diameter 4. Some eigenvalues are not integral.*

(ii) *Double Hoffman-Singleton Graph of diameter 5. Distinct eigenvalues are* $\{7, 3, 2, -2, -3, -7\}$.

(iii) *Double Gewirtz Graph of diameter 5. Distinct eigenvalues are* $\{10, 4, 2, -2, -4, -10\}$.

(iv) *Double 77-Graph of diameter 5. Distinct eigenvalues are* $\{16, 6, 2, -2, -6, -16\}$.

(v) *Double Higman-Sims Graph of diameter 5. Distinct eigenvalues are* $\{22, 8, 2, -2, -8, -22\}$.

(vi) *Dodecahedron of diameter 5. Distinct eigenvalues are not integer.*

3.3 Perfect state transfer on association schemes

Consider an association scheme $\{A_0, ..., A_d\}$. Any sum of distinct Schur idempotents is a 01-matrix and in particular defines a graph. We recall that we say that such a graph belongs to the association scheme. Our intent in this section is to construct new examples of perfect state transfer among such graphs.

3.3.1 Proposition. *If* A *and* B *are commuting matrices, then*

$$\exp(\mathtt{i}t(A + B)) = \exp(\mathtt{i}tA) \exp(\mathtt{i}tB).$$

□

We also recall two important facts in the following corollary (see Theorems 2.4.3 and 3.2.1).

3.3.2 Corollary. *If X is a graph belonging to an association scheme admitting perfect state transfer at time τ, then*

a) $U(\tau)$ is a multiple of a permutation matrix of order two and no fixed points that belongs to the Bose-Mesner algebra of the scheme; and

b) the eigenvalues of X are integers, and therefore $\tau = \frac{\pi}{g}$ for some integer g.

As a consequence, we can construct new examples of graphs admitting perfect state transfer based on old examples.

3.3.3 Corollary. *Suppose X is a graph belonging to an association scheme admitting perfect state transfer at time $\tau = \frac{\pi}{g}$ with phase λ. Let $A = A(X)$. Say $U(\tau) = \lambda T$. Let B be a 01-matrix belonging to the scheme satisfying the following properties.*

a) The 1s of B are in disjoint positions from those of A.

b) The eigenvalues of B are integers.

c) Either $|\theta|_2 = |g|_2$ for all eigenvalues θ of B, or $|\theta|_2 < |g|_2$ for all eigenvalues θ of B.

Then $A + B$ is the adjacency matrix of a graph, and $U_{A+B}(\tau) = \lambda' T$, where $\lambda' = \pm\lambda$.

Proof. From a), $A + B$ is the adjacency matrix of a graph. Conditions b) and c) imply that

$$U_B(\tau) = \pm \mathtt{I},$$

and so from Proposition 3.3.1, we have

$$U_{A+B}(\tau) = U_A(\tau) U_B(\tau) = \pm\lambda T.$$

□

A standard way of constructing association schemes is using the tensor product of matrices. We explain below.

Consider two association schemes $\{A_0, ..., A_d\}$ and $\{B_0, ..., B_e\}$. The set of matrices obtained by taking the Kronecker product of the matrices in both schemes

$$\{A_i \otimes B_j : \ 0 \leq i \leq d \text{ and } 0 \leq j \leq e\}$$

is an association scheme with $(de + d + e)$ classes (see Bailey [6, Chapter 3]). It is the *tensor product* of the original schemes.

The *direct product*[3] of graphs X and Y is defined to be the graph with adjacency matrix $A(X) \otimes A(Y)$, and is usually denoted by $X \times Y$. In Chapter 4, we will readdress the problem of characterizing perfect state transfer in graph products in a more general and detailed framework. Here we will present a particular case that provides a good number of examples of graphs belonging to association schemes admitting perfect state transfer.

The direct product of a graph X with K_2 is also referred to as the *bipartite double* of X. If X is distance-regular, $X \times K_2$ belongs to the tensor product of the schemes $\{\mathtt{I}, A(X), A_2(X), ..., A_d(X)\}$ and $\{\mathtt{I}_2, A(K_2)\}$.

3.3.4 Theorem. *Let $V(K_2) = \{v_1, v_2\}$. Suppose X is distance-regular on n vertices with eigenvalues $\theta_0 > ... > \theta_d$, and let $\theta_r = 2^{f_r}\ell_r$, where ℓ_r is an odd integer. For any vertex $u \in V(X)$, the graph $X \times K_2$ admits perfect state transfer between (u, v_1) and (u, v_2) if and only if both conditions hold:*

(i) For all r, we have $f_r = a$ for some constant a.

(ii) For all r and s, we have $\ell_r \equiv \ell_s \bmod 4$.

Under these conditions, perfect state transfer occurs at time $\frac{\pi}{2\gcd\{\theta_0,...,\theta_d\}}$.

Proof. It follows from the definition of direct product that the eigenvalues of $X \times K_2$ are $\pm\theta_i$. Note that the matrix $\mathtt{I}_n \otimes A(K_2)$ is a permutation matrix of order two having no fixed points, and that

$$(\mathtt{I}_n \otimes A(K_2))(E_{+\theta_i}) = E_{+\theta_i} \quad \text{and} \quad (\mathtt{I}_n \otimes A(K_2))(E_{-\theta_i}) = -E_{-\theta_i}.$$

Condition (iii) of Theorem 2.4.4 is equivalent to the two conditions below. Here g is the gcd of the differences of the eigenvalues of $X \times K_2$.

[3] See Section 4.2.

(1) $|\theta_r - \theta_s|_2 < |g|_2$ for all r and s; and

(2) $|\theta_r - (-\theta_s)|_2 = |g|_2$ for all r and s.

If $r = s$, then (2) is equivalent to Condition (i) of the statement. Assuming Condition (i), (1) and (2) are equivalent to

(1') $\frac{\ell_r - \ell_s}{2}$ even, for all r and s; and

(2') $\frac{\ell_r + \ell_s}{2}$ odd, for all r and s.

which is equivalent to Condition (ii). The time follows from the expression for time given in Theorem 2.4.4. □

The following corollaries are due to Coutinho et al. [21], and they exhibit some new examples of perfect state transfer. Note that the distance between vertices involved in perfect state transfer in these examples is the odd girth of the graph. The definition of these graphs can be found in Godsil and Royle [42, Chapter 10] for strongly regular graphs or in BCN [13] for distance-regular graphs. For generalized quadrangles, a more detailed account can be found in [61].

3.3.5 Corollary. *The following bipartite doubles of strongly regular graphs admit perfect state transfer.*

(i) Bipartite doubles of the point graphs of generalized quadrangles $GQ(s,t)$ whenever q is a prime power and one of the following conditions hold:

$$s = q-1, t = q+1 \textit{ with } q \equiv 0 \bmod 4,$$

$$s = q, t = q^2 \textit{ with } q \equiv 7 \bmod 8,$$

$$s = q^3, t = q^2 \textit{ with } q \equiv 7 \bmod 8,$$

$$t = 1 \ , \textit{ with } s \equiv 7 \bmod 8.$$

Number of vertices: $2(st+1)(s+1)$. Valency: $s(t+1)$. Perfect state transfer at $\frac{\pi}{4}$.

(ii) *Bipartite doubles of the complements of the point graphs of generalized quadrangles $GQ(s,t)$ whenever q is a prime power and one of the following conditions hold:*

$s = q, t = q^2$, *with* $q \equiv 3 \bmod 4$*: perfect state transfer at* $\frac{\pi}{2q}$,

$s = q^2, t = q$, *with* $q \equiv 3 \bmod 4$*: perfect state transfer at* $\frac{\pi}{2q}$,

$s = q-1, t = q+1$, *with* q *even : perfect state transfer at* $\frac{\pi}{2}$,

$s = q+1, t = q-1$, *with* q *even: perfect state transfer at* $\frac{\pi}{2}$,

$s = q^2, t = q^3$, *with* $q \equiv 3 \bmod 4$*: perfect state transfer at* $\frac{\pi}{2q^2}$,

$s = q^3, t = q^2$, *with* $q \equiv 3 \bmod 4$*: perfect state transfer at* $\frac{\pi}{2q^2}$.

Number of vertices: $2(st+1)(s+1)$*. Valency:* s^2t.

(iii) *Bipartite doubles of orthogonal array graphs* $OA(n,m)$ *if* $|n|_2 \leq \frac{|m|_2}{4}$*. Number of vertices:* $2n^2$*. Valency:* $m(n-1)$*. Perfect state transfer at* $\frac{2\pi}{\gcd(n,4m)}$.

(iv) *Bipartite doubles of complements of orthogonal array graphs* $OA(n,m)$ *if* $|n|_2 \leq \frac{m-1|_2}{4}$*. Number of vertices:* $2n^2$*. Valency:* $n^2 - m(n-1) - 1$*. Perfect state transfer at* $\frac{2\pi}{\gcd(n,4(m-1))}$.

3.3.6 Corollary. *The following bipartite doubles of distance-regular graphs with classical parameters admit perfect state transfer.*

(i) *Bipartite doubles of Grassmann graphs* $J_q(n,d)$ $(n \geq 2d)$ *for* n *even,* d *odd and* $q \equiv 3 \bmod 4$*. Classical parameters:* $\left(d, q, q, q\frac{q^{n-d}-1}{q-1}\right)$*. Perfect state transfer at* $\frac{\pi}{2}$.

(ii) *Bipartite doubles of Hamming graphs* $H(d,q)$ *when* $|q|_2 \leq |4d|_2$*. Classical parameters:* $(d,1,0,q-1)$*. Perfect state transfer at* $\frac{2\pi}{\gcd(q,4d)}$.

(iii) *Bipartite doubles of Doob graphs of odd diameter. Classical parameters:* $(d,1,0,3)$*. Perfect state transfer at* $\frac{\pi}{2}$.

(iv) *Bipartite doubles of unitary dual polar graphs* ${}^2A_{2d-1}(q)$ *and* ${}^2A_{2d}(q)$*, both cases when* $|q+1|_2 \leq |4d|_2$*. Classical parameters:* $(d,q^2,0,q)$ *and* $(d,q^2,0,q^3)$*, respectively. Perfect state transfer at* $\frac{2\pi}{\gcd(q+1,4d)}$.

(v) *Bipartite doubles of parabolic and symplectic dual polar graphs* $B_d(q)$ *and* $C_d(q)$ *when* $q \equiv 3 \bmod 4$ *and* d *is odd. Classical parameters:* $(d, q, 0, q)$. *Perfect state transfer at* $\frac{\pi}{2}$.

(vi) *Bipartite doubles of half dual polar graph of diameter* d *on* $2d$*-spaces when* $|q+1|_2 \leq |4d|_2$. *Classical parameters:* $\left(d, q^2, q^2+q, q\frac{q^{2d-1}-1}{q-1}\right)$. *Perfect state transfer at* $\frac{\pi}{2\gcd(d,q+1)}$.

(vii) *Bipartite doubles of half dual polar graph of diameter* d *on* $2d+1$*-spaces when* $|(q+1)(q^2+1)|_2 \leq |4d|_2$. *Classical parameters:* $\left(d, q^2, q^2+q, q\frac{q^{2d+1}-1}{q-1}\right)$. *Perfect state transfer at*

$$\frac{2\pi}{\gcd\left((q+1)(q^2+1), 4\frac{q^{2d+1}-1}{q^2-1}\frac{q^{2d}-1}{q-1}\right)}.$$

(viii) *Bipartite doubles of exceptional graphs of Lie type when* $q \equiv 11 \bmod 12$ *or when* $q \equiv 3, 7 \bmod 12$. *Classical parameters:* $\left(3, q^4, q\frac{q^4-1}{q-1}, q\frac{q^9-1}{q-1}\right)$. *In the first case, perfect state transfer at time* $\frac{\pi}{6}$. *In the second, at time* $\frac{\pi}{2}$.

(ix) *Bipartite doubles of all affine* E_6 *graphs when* q *is even. Classical parameters:* $(3, q^4, q^4-1, q^9-1)$. *Perfect state transfer at* $\frac{\pi}{2}$.

(x) *Bipartite doubles of all alternating forms graphs when* q *is even. Classical parameters:* $(d, q^2, q^2-1, q^{2d-1}-1)$ *and* $(d, q^2, q^2-1, q^{2d+1}-1)$ *for forms on* $2d$*- and on* $2d+1$*-spaces, respectively. Perfect state transfer at* $\frac{\pi}{2}$.

(xi) *Bipartite doubles of all Hermitian forms graphs when* q *is even. Classical parameters:* $(d, -q, -q-1, -(-q)^d-1)$. *Perfect state transfer at* $\frac{\pi}{2}$.

Chapter 4

Graph products and double-covers

This chapter examines in detail how perfect state transfer in certain graph products relates to properties of the factors. The methods we introduce in this chapter can be used to study state transfer in graphs whose adjacency matrix is a sum of Kronecker products of matrices.

First, we present an overview of our methods, restricting to the case in which the adjacency matrix of the graph X is of the form

$$A(X) = B \otimes C + M \otimes N$$

with B, C, M, N symmetric matrices. All significant examples we have are graphs of this form.

Following this, we study in detail perfect state transfer in the direct product of graphs. This problem was studied by Ge et al. [31]. In particular, they showed that $X \times H$ admits perfect state transfer if X admits perfect state transfer at a time τ, $\frac{\tau\theta}{\pi} \in \mathbb{Z}$ for all eigenvalues θ of X, and H is a circulant graph with odd eigenvalues. Here we will generalize their work. On one hand, we first show that if $X \times Y$ admits perfect state transfer, then at least one of the factors must admit perfect state transfer (similarly to what happens with the Cartesian product of graphs). On the other hand, we show that the hypothesis on the other factor can be significantly weakened, in particular, H need not be a circulant nor have odd eigenvalues. For example, we show that under somewhat similar integrality conditions on the eigenvalues, if X admits perfect state transfer and the 2-adic norm of the integer part of the eigenvalues of Y is constant, then $X^{\square k} \otimes Y$ admits perfect state transfer for some sufficiently large values of k.

We then proceed to show how our methods can be used in other notions of graph products, in particular, we will show that the sufficient condition for perfect state transfer in the lexicographic product of regular graphs presented by Ge et al. [31] is also necessary. We will also show that perfect state transfer in the strong product of graphs can be determined using the same methods we used for the direct product.

Finally, we will apply our methods to graphs which are double-covers of other graphs, focusing on double-covers of the complete graph. Here we will find new examples of perfect state transfer.

4.1 Framework for studying state transfer in products

In this section, we will introduce a very general method for determining whether perfect state transfer is possible in graphs which are sums of tensor products of 01-matrices. For the purpose of simplifying the notation, we will restrict our considerations to graphs X such that

$$A(X) = B \otimes C + M \otimes N$$

with B, C, M, N symmetric matrices, but both the number of terms of the sum and the number of factors in each term can be generalized to any positive integer, as we will see in Section 4.3.

Definition. The *Cartesian product* of graphs X and Y is denoted by $X \square Y$ and is defined as the graph with adjacency matrix

$$A(X \square Y) = A(X) \otimes \mathtt{I} + \mathtt{I} \otimes A(Y).$$

It can be defined combinatorially as follows. Its vertex set is $V(X \square Y) = V(X) \times V(Y)$, and $(u_1, v_1) \sim (u_2, v_2)$ if and only if either $u_1 = u_2$ and $v_1 v_2 \in E(Y)$, or $v_1 = v_2$ and $u_1 u_2 \in E(X)$. Thus $A(X \square Y)$ and $A(Y \square X)$ define the same graph.

4.1.1 Theorem (Christandl et al. [20]). *If X and Y are graphs, then, for all t, we have*

$$U_{X\square Y}(t) = U_X(t) \otimes U_Y(t). \tag{4.1}$$

We will later present a proof of Theorem 4.1.1, but note that it implies the following corollary trivially.

4.1.2 Corollary. *For graphs X and Y, the graph $X\square Y$ admits perfect state transfer at time τ if and only if either of the graphs admits perfect state transfer at time τ, and if only one of them does, the other must contain a vertex which is periodic at time τ.*

When we introduced the spectral decomposition of a matrix, we assumed the projectors E_r represent projections onto the eigenspaces, and therefore their ranks are equal to the multiplicity of the corresponding eigenvalues. Now we consider a refinement of such a decomposition. If M is a symmetric $m \times m$ matrix, M admits a decomposition into rank-1 orthogonal projectors

$$M = \sum_{r=0}^{m-1} \theta_r E_r. \tag{4.2}$$

Here we are no longer requiring that $\theta_r \neq \theta_s$ if $r \neq s$. Note that if $\{\mathbf{v}_0, ..., \mathbf{v}_{m-1}\}$ forms an orthonormal basis of eigenvectors of M, then we can choose $E_r = \mathbf{v}_r \mathbf{v}_r^T$.

For the lemmas below, suppose X is such that $A(X) = B \otimes C + M \otimes N$. We require B and M to be $m \times m$ matrices, and C and N to be $n \times n$ matrices. Because of that, we identify the rows and columns of B and M, similarly for C and N. A typical vertex of X will be represented as (w, u), where w indexes a row of B and M, and u a row of C and N. Further to that, suppose that B and M commute. Let $\beta_0 \geq ... \geq \beta_{m-1}$ and $\mu_0 \geq ... \geq \mu_{m-1}$ be the spectra of B and M respectively, and $\gamma_0 \geq ... \geq \gamma_{n-1}$ and $\nu_0 \geq ... \geq \nu_{n-1}$ be the spectra of C and N respectively.

4.1.3 Lemma. *Suppose X is as above. Then $U_X(t)$ is similar to a block diagonal matrix with m blocks, in which each block is of the form $\exp(\mathtt{i}tL_r)$, with*

$$L_r = \beta_r C + \mu_r N.$$

Proof. By Theorem 2.1.8, and because B and M are symmetric and commute, there exists an orthogonal matrix P such that $P^T BP$ and $P^T MP$ are diagonal. Hence we have that

$$L = (P^T \otimes \mathtt{I})\,(B \otimes C + M \otimes N)\,(P \otimes \mathtt{I})$$

is a block diagonal matrix whose blocks are equal to $L_r = \beta_r C + \mu_r N$. The result now follows from the fact that

$$U_L(t) = (P^T \otimes \mathtt{I})\; U_X(t)\; (P \otimes \mathtt{I}).$$

□

In the context of the lemma above, we recall that we can use the terms *perfect state transfer* and *periodicity* with respect to symmetric matrices in general.

4.1.4 Lemma. *Suppose X is as above, and let $E_0, ..., E_{m-1}$ be the rank-1 projectors onto the common eigenspaces of B and M. Let $L_r = \beta_r C + \mu_r N$. If the graph X admits perfect state transfer from (w, u) to (z, v), then*

(i) the vertices (column indices) w and z are strongly cospectral in the matrices B and M; and

(ii) for all r such that $E_r w \neq \mathbf{0}$; if $u = v$, the matrix L_r is periodic at u; and if $u \neq v$, the matrix L_r admits perfect state transfer from u to v.

Proof. By hypothesis, there exists a time τ and a complex number λ such that

$$U_X(\tau)(\mathbf{e}_w \otimes \mathbf{e}_u) = \lambda(\mathbf{e}_z \otimes \mathbf{e}_v).$$

Let P be the matrix that simultaneously diagonalizes B and M. Hence

$$(P^T \otimes I)U_X(\tau)(\mathbf{e}_w \otimes \mathbf{e}_u) = \lambda(P^T \mathbf{e}_z \otimes \mathbf{e}_v),$$

and thus, by Lemma 4.1.3,

$$\begin{pmatrix} \mathsf{e}^{\mathtt{i}\tau L_0} & & & \\ & \mathsf{e}^{\mathtt{i}\tau L_2} & & \\ & & \ddots & \\ & & & \mathsf{e}^{\mathtt{i}\tau L_{m-1}} \end{pmatrix} (P^T \mathbf{e}_w \otimes \mathbf{e}_u) = \lambda(P^T \mathbf{e}_z \otimes \mathbf{e}_v).$$

This is true if and only if, for all $r = 0, ..., m-1$,

$$(\mathbf{e}_r^T P^T \mathbf{e}_w)\mathsf{e}^{\mathtt{i}\tau L_r}\mathbf{e}_u = (\mathbf{e}_r^T P^T \mathbf{e}_z)\lambda \mathbf{e}_v.$$

Because the matrices $\mathsf{e}^{\mathtt{i}tL_r}$ are all unitary, it follows that, for all r,

$$(\mathbf{e}_r^T P^T \mathbf{e}_w) = \pm(\mathbf{e}_r^T P^T \mathbf{e}_z),$$

and so w and z are strongly cospectral in the matrices B and M; and also that

$$\mathsf{e}^{\mathtt{i}\tau L_r}\mathbf{e}_u = \pm\lambda \mathbf{e}_v$$

for all r such that $(\mathbf{e}_r^T P^T \mathbf{e}_w) \neq 0$. □

4.1.5 Lemma. *Suppose X is as above, and now with the extra assumption that C and N also commute. Let $F_0, ..., F_{n-1}$ be the common rank-1 projectors for C and N. Then*

$$U_X(t) = \sum_{r=0}^{m-1}\sum_{s=0}^{n-1} \mathsf{e}^{\mathtt{i}t(\beta_r\gamma_s + \mu_r\nu_s)} E_r \otimes F_s.$$

Proof. Note that

$$B \otimes C + M \otimes N = \sum_{r=0}^{m-1}\sum_{s=0}^{n-1} (\beta_r\gamma_s + \mu_r\nu_s) E_r \otimes F_s.$$

From

$$U_X(t) = \exp\Big(\mathtt{i}t\big(B \otimes C + M \otimes N\big)\Big),$$

and the facts that $BM = MB$ and $CN = NC$, it follows that

$$U_X(t) = \sum_{r=0}^{m-1}\sum_{s=0}^{n-1} \mathsf{e}^{\mathtt{i}t(\beta_r\gamma_s + \mu_r\nu_s)} E_r \otimes F_s.$$

□

4.2 Direct product of graphs

Consider graphs X and Y with respective adjacency matrices $A(X)$ and $A(Y)$.

Definition. We recall that the *direct product* of X and Y, denoted by $X \times Y$, is the graph with adjacency matrix $A(X) \otimes A(Y)$.

It can be defined combinatorially as follows. Its vertex set is $V(X \times Y) = V(X) \times V(Y)$, and $(u_1, v_1) \sim (u_2, v_2)$ if and only if $u_1 u_2 \in E(X)$ and $v_1 v_2 \in E(Y)$. Thus $A(X) \otimes A(Y)$ and $A(Y) \otimes A(X)$ define the same graph.

This product is also known in the literature as the weak direct product, the tensor product, the categorical product, and many other names (see Hammack et al. [46, Chapter 4]). In this section, we study when a direct product of graphs admits perfect state transfer. As an immediate application, we find more examples of perfect state transfer.

4.2.1 Theorem. *Suppose X and Y are graphs, and $X \times Y$ admits perfect state transfer between vertices (w, u) and (z, v). If $u = v$, then Y is periodic at u. If $u \neq v$, then Y admits perfect state transfer between u and v. Likewise, if $w = z$, then X is periodic at w. If $w \neq z$, then X admits perfect state transfer between w and z.*

Proof. It is a simple consequence of Lemma 4.1.4 with $B = C = \mathtt{0}$, $M = A(X)$ and $N = A(Y)$, or $M = A(Y)$ and $N = A(X)$. □

4.2.2 Lemma. *Suppose X and Y are graphs and $A(X)$ admits the spectral decomposition $A(X) = \sum_{r=0}^{d} \theta_r E_r$. Then*

$$U_{X \times Y}(t) = \sum_{r=0}^{d} E_r \otimes U_Y(\theta_r t).$$

Proof. It is a consequence of Lemma 4.1.5 and an easy rearrangement. □

Now we will show under which conditions on the factors we can obtain perfect state transfer on the product.

4.2.3 Theorem. *Suppose $U_Y(\tau)\boldsymbol{e}_u = \lambda \boldsymbol{e}_v$, and that the eigenvalues of Y in the support of u are of the form $b_i\sqrt{\Delta_u}$. Suppose w and z are strongly cospectral vertices in X. Then $X \otimes Y$ admits perfect state transfer from (w, u) to (z, v) if and only if the following conditions hold.*

(i) For all $\theta_r \in \Phi_w$, we have $\theta_r = t_r\sqrt{\Delta_w}$, where $t_r \in \mathbb{Z}$ and Δ_w is a square-free positive integer (which could be 1).

(ii) The 2-adic norms of t_r are all the same.

(iii) If λ is a primitive n-th root of the unit, then n is even, and there exists an integer m such that

a) If $\theta_r \in \Phi^+_{wz}$, then the odd part of t_r is congruent to m modulo n.

b) If $\theta_r \in \Phi^-_{wz}$, then the odd part of t_r is congruent to $m + \frac{n}{2}$ modulo n.

Proof. Let $\Phi_w = \{\theta_0, ..., \theta_d\}$, and $\Phi_u = \{\varphi_0, ..., \varphi_k\}$. Let h be the gcd of the differences $(\varphi_0 - \varphi_r)$ for $r = 1, ..., k$. Let $h = 2^e\ell$, with ℓ an odd integer.

Suppose that perfect state transfer occurs in $X \times Y$ between (w, u) and (z, v) at time τ and phase γ. As a consequence of the fact that $A(X \times Y) = A(X) \otimes A(Y)$, the eigenvalues in the support of (w, u) are of the form $\theta_r\varphi_i$, with $0 \leq r \leq d$ and $0 \leq i \leq k$. In light of Theorem 2.4.3, the eigenvalues θ_r are either integers or integer multiples of $\sqrt{\Delta_w}$ for some square-free positive $\Delta_w \in \mathbb{Z}$.

Then, using Lemma 4.2.2, we have

$$\begin{aligned}\gamma(\mathbf{e}_z \otimes \mathbf{e}_v) &= U_{X\otimes Y}(\tau)(\mathbf{e}_w \otimes \mathbf{e}_u)\\ &= \sum_{r=0}^{d}(E_r \otimes U_Y(\theta_r\tau))(\mathbf{e}_w \otimes \mathbf{e}_u)\\ &= \sum_{r=0}^{d} E_r\mathbf{e}_w \otimes U_Y(\theta_r\tau)\mathbf{e}_u.\end{aligned}$$

Multiplying both sides by $E_r \otimes \mathtt{I}$, we get that, for $\sigma_r \in \{+1, -1\}$,

$$U_Y(\theta_r\tau)\mathbf{e}_u = \sigma_r\gamma\mathbf{e}_v$$

depending on whether $\theta_r \in \Phi^+_{wz}$ of $\theta_r \in \Phi^-_{wz}$. In either case, $\theta_r\tau$ is a time for which perfect state transfer occurs in Y between u and v. Applying Theorem 2.4.4, this implies that

$$\theta_r\tau = \ell_r \frac{\pi}{2^e.\ell\sqrt{\Delta_u}} \quad \text{and} \quad \sigma_r\gamma = \lambda^{\ell_r},$$

where ℓ_r is an odd integer. Considering θ_r and θ_s in the support of w, we will have

$$\frac{\theta_r}{\theta_s} = \frac{\ell_r}{\ell_s}. \tag{4.3}$$

Because the integers ℓ_r are odd, the 2-adic norm of each t_r is the same, proving (ii).

To prove condition (iii), suppose we take $m' \in \{1, ..., n\}$ such that $\lambda^{m'} = \gamma$. The fact that there is a m'' such that $\lambda^{m''} = -\gamma$ is equivalent to (-1) being a power of λ, which happens if and only if n is even. In that case, if $\theta_r \in \Phi^+_{wz}$, then $\ell_r \equiv m' \bmod n$, and if $\theta_r \in \Phi^-_{wz}$, then $\ell_r \equiv m' + \frac{n}{2} \bmod n$. Note that the odd part of t_r is an odd multiple ℓ_r, which by Equation 4.3 does not depend on r. Say ℓ'. So if the integers ℓ_r satisfy the congruences with m', so will the odd parts of t_r with $m = m'\ell'$.

Now suppose all three conditions hold. Let $t_r = 2^f.k_r$, for some $f \geq 0$ and odd integers k_r. By Lemma 4.2.2, we have

$$U_{X\times Y}\left(\frac{\pi}{2^{e+f}\ell\sqrt{\Delta_w}\sqrt{\Delta_u}}\right) = \sum_{r=0}^{d} E_r \otimes U_Y\left(\theta_r.\frac{\pi}{2^{e+f}\ell\sqrt{\Delta_w}\sqrt{\Delta_u}}\right).$$

Note that

$$\begin{aligned} U_Y\left(\theta_r.\frac{\pi}{2^{e+f}\ell\sqrt{\Delta_w}\sqrt{\Delta_u}}\right) &= U_Y\left(k_r\frac{\pi}{2^e\ell\sqrt{\Delta_u}}\right) \\ &= \left[U_Y\left(\frac{\pi}{2^e\ell\sqrt{\Delta_u}}\right)\right]^{k_r} \end{aligned}$$

Hence

$$\begin{aligned} U_{X\times Y}\left(\frac{\pi}{2^{e+f}\ell\sqrt{\Delta_w}\sqrt{\Delta_u}}\right)(\mathbf{e}_w \otimes \mathbf{e}_u) &= \sum_{r=0}^{d} E_r\mathbf{e}_w \otimes \left[U_Y\left(\frac{\pi}{2^e\sqrt{\Delta_u}}\right)\right]^{k_r}\mathbf{e}_u \\ &= \sum_{r=0}^{d} E_r\mathbf{e}_w \otimes \lambda^{k_r}\mathbf{e}_v. \end{aligned}$$

If $r \in \Phi_{wz}^{+}$, then condition (iii) implies that $\lambda^{k_r} = \lambda^m$, and if $r \in \Phi_{wz}^{-}$, then $\lambda^{k_r} = \lambda^{-m}$. If $\lambda^m = \gamma$, we have

$$U_{X\times Y}\left(\frac{\pi}{2^{e+f}\sqrt{\Delta_w}\sqrt{\Delta_u}}\right)(\mathbf{e}_w \otimes \mathbf{e}_u) = \gamma(\mathbf{e}_z \otimes \mathbf{e}_v),$$

as claimed. □

Note that if $w = z$, the theorem above takes the following form.

4.2.4 Corollary. *Suppose $U_Y(\tau)\boldsymbol{e}_u = \lambda \boldsymbol{e}_v$, and that the eigenvalues of Y in the support of u are of the form $b_i\sqrt{\Delta_u}$. Let $w \in V(X)$. Then $X \times Y$ admits perfect state transfer from (w,u) to (w,v) if and only if the following conditions hold.*

(i) For all $\theta_r \in \Phi_w$, we have $\theta_r = t_r\sqrt{\Delta_w}$, where $t_r \in \mathbb{Z}$ and Δ_w is a square-free positive integer (which could be 1).

(ii) The 2-adic norms of t_r are all the same.

(iii) If λ is a primitive n-th root of the unit, then there exists an integer m such that the odd part of the integer t_r is congruent to m modulo n.

We draw the reader's attention to the following fact. The conditions on X of both results depend very little on Y. In fact, if φ_0 is the largest eigenvalue of Y and τ is the time at which perfect state transfer occurs in Y, then the three conditions depend only on the eigenvalues of X, with the exception of the order of $\mathrm{e}^{\mathrm{i}\varphi_0\tau}$ as a root of unity. This fact can be explored in the following corollary.

4.2.5 Corollary. *If $X \times Y$ admits perfect state transfer, and if the eigenvalues of Y in the support of the vertices involved in perfect state transfer are integers or integer multiples of a square root, then $X \times Y^{\square k}$ admits perfect state transfer for all $k \in \mathbb{Z}^+$.*

Proof. By Theorem 4.1.1, if Y admits perfect state transfer at minimum time τ, then so does $Y^{\square k}$ at the same time. Moreover, if the largest eigenvalue of Y is φ_0, then the largest eigenvalue of $Y^{\square k}$ is $k\varphi_0$. Hence the order of the phase of state transfer in $Y^{\square k}$

either decreases or stays the same. If it decreases by an odd factor, nothing changes. If it decreases by an even factor, then what could happen is that $X \times Y$ admits perfect state transfer between (w, u) and (z, v) and $X \times Y^{\square k}$ admits perfect state transfer between $(w, u, u, ..., u)$ and $(w, v, v, ..., v)$, and between $(z, u, u, ..., u)$ and $(z, v, v, ..., v)$. $\square$

This can be pushed even further.

4.2.6 Corollary. *If Y admits perfect state transfer, if the eigenvalues of X and Y are integers or integer multiples of a square root, and if the 2-adic norm of the integer parts of the eigenvalues of X are all the same, then there exists a $k_0 \in \mathbb{Z}^+$ such that $X \otimes Y^{\square(mk_0)}$ admits perfect state transfer for all $m \geq 1$.*

As a consequence, we present new examples of perfect state transfer in simple graphs. For the cases below, we assume that Y is a graph admitting perfect state transfer between u and v, and that the eigenvalues of Y in the support of u are either integers or integer multiples of square roots. All the graphs known in the literature admitting perfect state transfer are of this form.

Example 6 (**Stars**). Let S_n represent the graph on $n+1$ vertices with degree sequence $(n, 1, 1, ..., 1)$. The spectrum of S_n is

$$\{\sqrt{n}^{(1)},\ 0^{(n-2)},\ -\sqrt{n}^{(1)}\}.$$

Let w be the vertex of degree n. The eigenvalue support of w is $\{\sqrt{n}, -\sqrt{n}\}$.

From Corollary 4.2.6, there is a k such that $S_n \times Y^{\square k}$ admits perfect state transfer from $(w, u, u, ..., u)$ to $(w, v, v, ..., v)$.

Note that k is usually quite small. If Y admits perfect state transfer at time $\frac{\pi}{2}$, which is a rather common situation, then $k = 2$ will suffice.

Example 7 (**Odd eigenvalues**). If X is a graph with odd eigenvalues, and $w \in V(X)$, then it follows from Corollary 4.2.6 that there is a k such that $X \times Y^{\square k}$ admits perfect state transfer from $(w, u, u, ..., u)$ to $(w, v, v, ..., v)$.

We can find many graphs with odd eigenvalues among the known distance-regular graphs. For example, there are 32548 non-isomorphic strongly regular graphs with parameters (36,15,6,6). These graphs have eigenvalues $\{15, 3, -3\}$. The tensor product of each of them with C_4 will admit perfect state transfer.

4.3 Other graph products

We list some examples of traditional graph products below. See Hammack et al. [46] for the combinatorial definitions.

1) The *lexicographic product* $X \wr Y$ satisfies

$$A(X \wr Y) = A(X) \otimes \mathtt{J} \ + \ \mathtt{I} \otimes A(Y).$$

2) The *strong graph product* $X \boxtimes Y$ satisfies

$$A(X \boxtimes Y) = A(X) \otimes [A(Y) + \mathtt{I}] \ + \ \mathtt{I} \otimes A(Y).$$

3) The *modular product* $X \diamond Y$ satisfies

$$A(X \diamond Y) = A(X) \otimes [A(Y) + \mathtt{I}] \ + \ \mathtt{I} \otimes A(Y) \ + \ A(\overline{X}) \otimes A(\overline{Y}).$$

The matrix $A(X)$ commutes with $\mathtt{I}$, and so we can use the technology from Section 4.1 to analyse cases 1) and 2). Our technology could also be applied to study case 3) if we assume that either X or Y is regular.

For the lexicographic product $X \wr Y$, we further suppose that Y and $\mathtt{J}$ commute, which is equivalent to Y being a k-regular graph. If $A(X)$ and $A(Y)$ admit decompositions into rank-1 projectors

$$A(X) = \sum_{r=0}^{n-1} \theta_r E_r \quad \text{and} \quad A(Y) = \frac{k}{m}\mathtt{J} + \sum_{s=1}^{m-1} \rho_s F_s,$$

then it follows from Lemma 4.1.5 that

$$U_{X\wr Y}(t) = \sum_{r=0}^{n-1}\left(\mathtt{e}^{\mathtt{i}t(\theta_r m+k)} E_r \otimes \frac{1}{m}\mathtt{J} + \sum_{s=1}^{m-1} \mathtt{e}^{\mathtt{i}t\rho_s} E_r \otimes F_s\right),$$

and so

$$U_{X\wr Y}(t) = U_X(mt)\otimes \frac{\mathtt{e}^{\mathtt{i}tk}}{m}\mathtt{J} \;+\; \mathtt{I}\otimes\left(U_Y(t) - \frac{\mathtt{e}^{\mathtt{i}tk}}{m}\mathtt{J}\right). \tag{4.4}$$

In Ge et al. [31, Lemma 5], sufficient conditions for perfect state transfer in $X\wr Y$ when Y is regular are presented. Here we characterize perfect state transfer in this context.

4.3.1 Theorem. *Suppose X and Y are graphs, and Y is k-regular on m vertices, $m > 1$. Then $X \wr Y$ admits perfect state transfer from (u, w) to (v, z) at time τ and with phase λ if and only the conditions below hold.*

(i) X is periodic at u at time $m\tau$ with a phase γ.

(ii) The vertices w and z are distinct and strongly cospectral in Y.

(iii) The following equality holds $\gamma\mathtt{e}^{\mathtt{i}\tau k} = \lambda$.

(iv) For all $s \in \{1, ..., m-1\}$, we have $\mathtt{e}^{\mathtt{i}\tau\rho_s} F_s \boldsymbol{e}_w = \lambda F_s \boldsymbol{e}_z$.

Proof. By Equation 4.4, $U_{X\wr Y}(\tau)(\mathbf{e}_u \otimes \mathbf{e}_w) = \lambda(\mathbf{e}_v \otimes \mathbf{e}_z)$ if and only if

$$(U_X(m\tau) - \mathtt{I})\mathbf{e}_u \otimes \frac{\mathtt{e}^{\mathtt{i}\tau k}}{m}\mathbf{j} \;+\; \mathbf{e}_u \otimes U_Y(\tau)\mathbf{e}_w = \lambda(\mathbf{e}_v \otimes \mathbf{e}_z).$$

This is equivalent to having $\mathbf{e}_u = \mathbf{e}_v$, and to existing a γ such that $U_X(m\tau)\mathbf{e}_u = \gamma\mathbf{e}_u$ and

$$U_Y(\tau)\mathbf{e}_w = \lambda\mathbf{e}_z - \frac{(\gamma-1)}{m}\mathtt{e}^{\mathtt{i}\tau k}\mathbf{j}.$$

This equality above is true if and only if the projections of both sides on each eigenspace of $A(Y)$ are equal. For the eigenspaces that do not correspond to the eigenvalue k, the projections are equal if and only if conditions (ii) and (iv) hold. The projections onto the eigenspace corresponding to k are equal if and only if

$$(\gamma - 1)\mathtt{e}^{\mathtt{i}\tau k} + \mathtt{e}^{\mathtt{i}\tau k} = \lambda,$$

or equivalently $\gamma\mathtt{e}^{\mathtt{i}\tau k} = \lambda$. $\square$

Example 8. Using the result above, we can construct a new example of perfect state transfer. Consider the lexicographic product $K_2 \wr \overline{(mK_2)}$ with m odd. In this case, $\tau = \frac{\pi}{2}$, $\gamma = -1$ and $\lambda = -1$.

For the strong graph product, we have the following.

4.3.2 Proposition. *If X and Y are graphs, and $A(X) = \sum_{r=0}^{d} \theta_r E_r$ is the spectral decomposition of $A(X)$ with θ_r varying among its distinct eigenvalues, we have:*

$$U_{X \boxtimes Y}(t) = \sum_{r=0}^{d} \mathtt{e}^{\mathtt{i}\theta_r t} E_r \otimes U_Y((\theta_r + 1)t).$$

Proof. We split the expression for the strong product as

$$A(X \boxtimes Y) = A(X) \otimes \mathtt{I} + \mathtt{I} \otimes A(Y) + A(X) \otimes A(Y),$$

or even

$$A(X \boxtimes Y) = A(X \square Y) + A(X \times Y).$$

Thus

$$U_{X \boxtimes Y}(t) = U_{X \square Y}(t) \cdot U_{X \times Y}(t),$$

and hence, using Lemma 4.2.2 and Theorem 4.1.1,

$$\begin{aligned} U_{X \boxtimes Y}(t) &= \big(U_X(t) \otimes U_Y(t)\big)\Big(\sum_{r=0}^{d} E_r \otimes U_Y(\theta_r t)\Big) \\ &= \sum_{r=0}^{d} \mathtt{e}^{\mathtt{i}\theta_r t} E_r \otimes U_Y((\theta_r + 1)t). \end{aligned}$$

□

The corollary below is an analogous version of Theorem 4.2.1 and it is a straightforward consequence of Lemma 4.1.4.

4.3.3 Corollary. *Suppose X and Y are graphs, $A(X) = \sum_{r=0}^{d} \theta_r E_r$, and $X \boxtimes Y$ admits perfect state transfer between vertices (w, u) and (z, v). If $u = v$, then Y is periodic at u. If $u \neq v$, then Y admits perfect state transfer between u and v. Likewise, if $w = z$, then X is periodic at w. If $w \neq z$, then X admits perfect state transfer between w and z.*

Moreover, analogous results to Theorem 4.2.3 and Corollary 4.2.4 could be written in this case, but with more complicated expressions.

4.4 Double-covers and switching graphs

Definition. Given graphs X and Y on the same set of vertices, we define the graph $X \ltimes Y$ as the graph with adjacency matrix

$$A(X \ltimes Y) = \begin{pmatrix} A(X) & A(Y) \\ A(Y) & A(X) \end{pmatrix}.$$

If $A(X) \circ A(Y) = \mathtt{0}$, then $X \ltimes Y$ is a *double cover* of the graph with adjacency matrix $A(X) + A(Y)$. When $A(Y) = \mathtt{J} - \mathtt{I} - A(X)$, then $X \ltimes Y$ is a double cover of the complete graph and is known in the literature as the *switching graph* of X (see Godsil and Royle [42, Chapter 11]).

If X is the empty graph, then $X \ltimes Y = A(K_2) \otimes A(Y)$ is the *bipartite double* of Y. We studied perfect state transfer on bipartite doubles of graphs belonging to association schemes in Section 3.3. Here we intend to study $X \ltimes Y$ in a more general form.

Note that $\mathtt{I}_2$ and $A(K_2)$ commute, and can be simultaneously diagonalized by

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Using Lemma 4.1.3, we have the following lemma.

4.4.1 Lemma. *Given graphs X and Y, with $A = A(X)$ and $B = A(Y)$, we have, for all t,*

$$(H \otimes I) U_{X \ltimes Y}(t) (H \otimes I) = \begin{pmatrix} U_{A+B}(t) & 0 \\ 0 & U_{A-B}(t) \end{pmatrix}.$$

4.4.2 Theorem. *Given graphs X and Y on the same vertex set V, with $A = A(X)$ and $B = A(Y)$, the graph $X \ltimes Y$ on vertex set $\{0, 1\} \times V$ admits perfect state transfer if and only if, for some $\tau \in \mathbb{R}+$ and $u \in V$,*

$$\lambda = [U_{A+B}(\tau)]_{u,u} = -[U_{A-B}(\tau)]_{u,u} \quad \textit{and} \quad |\lambda| = 1.$$

In that case, perfect state transfer is between $(0,u)$ *and* $(1,u)$.

Proof. From Lemma 4.4.1, it follows that

$$U_{X\ltimes Y}(t) = \frac{1}{2}\begin{pmatrix} U_{A+B}(t)+U_{A-B}(t) & U_{A+B}(t)-U_{A-B}(t) \\ U_{A+B}(t)-U_{A-B}(t) & U_{A+B}(t)+U_{A-B}(t) \end{pmatrix}.$$

For any $u \in V$, if perfect state transfer happens at τ between $(0,u)$ and some other vertex, then $[U_{A+B}(\tau)+U_{A-B}(\tau)]_{u,u} = 0$. Hence

$$\lambda = [U_{A+B}(\tau)]_{u,u} = -[U_{A-B}(\tau)]_{u,u}.$$

This implies that the u-th diagonal entry of $U_{A+B}(t) - U_{A-B}(t)$ is non-zero. It will be a complex number of order 1 if and only if $|\lambda| = 1$. □

4.4.3 Corollary. *Let* $\theta_0 > \ldots > \theta_d$ *be the eigenvalues of* $A(X) - A(\overline{X})$. *Suppose* $|V(X)| = n > 2$. *Then* $X \ltimes \overline{X}$ *admits perfect state transfer if and only if* n *is even and for all* θ_r *in the support of a vertex* u, *the number* $(\theta_r + 1)$ *is an integer, and the* 2*-adic norm of each* $(\theta_r + 1)$ *is always the same.*

Proof. Let $A = A(X)$ and $B = A(\overline{X})$. Let $\lambda = [U_{A+B}(\tau)]_{u,u}$. Because $A + B = \mathtt{J} - \mathtt{I}$, it follows that $|\lambda| = 1$ if and only if $\tau = \frac{2k\pi}{n}$. In that case, $\lambda = \mathtt{e}^{-\mathtt{i}\tau}$. Given Lemma 4.4.2, perfect state transfer between $(0,u)$ and $(1,u)$ happens if and only if

$$\mathtt{e}^{\mathtt{i}\tau\theta_r} = \mathtt{e}^{-\mathtt{i}\tau}$$

for all θ_r in the support of u. This is equivalent to the condition in the statement. □

If $A = A(X)$ and $B = A(Y)$ commute, then $U_{A\pm B}(t) = U_A(t)U_B(\pm t)$, and we have the easy characterization of perfect state transfer in $A \ltimes Y$ below.

4.4.4 Corollary. *Suppose* $A = A(X)$ *and* $B = A(Y)$ *commute. Then perfect state transfer happens in* $X \ltimes Y$ *between* $(0,u)$ *and* $(1,u)$ *if and only if there is a time* τ *such that* X *is periodic at* u *at time* τ, *and* Y *is periodic at* u *at time* τ *and with phase* $\pm\mathtt{i}$.

We use the corollary above to show some new examples of perfect state transfer.

Example 9 (Switching graphs). The graph $K_n \square K_n$ is a strongly regular graph with parameters $(n^2, 2n-2, n-2, 2)$. Its eigenvalues are $\{2n-2,\ n-2,\ -2\}$, hence for all n divisible by 4, it follows from Corollary 4.4.4 that the switching graph of $K_n \square K_n$ admits perfect state transfer at time $\frac{\pi}{2}$.

There are two feasible parameter sets for strongly regular graphs on 96 vertices for which constructions of such graphs are known (see [15]). The parameter sets are $(96, 20, 4, 4)$ and $(96, 76, 60, 60)$. One example for the first set is the point-graph of the generalized quadrangle GQ(5,3). The switching graphs of all strongly regular graphs with such parameters admit perfect state transfer.

Chapter 5

Translation graphs

This chapter is motivated by the following problem of characterizing which translation graphs[1] admit perfect state transfer, which we are quite far from solving.

We examine the work of Godsil and others on cubelike graphs, and the work of Bašić and others on circulant graphs. In the former case, perfect state transfer on cubelike graphs at time $\frac{\pi}{2}$ was fully characterized, thus our aim is to find more explicit results on perfect state transfer at shorter times, particularly at times less than $\frac{\pi}{4}$. Our main contribution in this section is the observation that perfect state transfer at shorter times is related to the concept of uniform mixing in quantum walks. In the latter, even though perfect state transfer is fully characterized for circulant graphs, we examine the problem using a different technique. Our immediate goal is to find simpler proofs of known results, but we were only able to compute the time at which perfect state transfer occurs in a more explicit way than was originally done. These two sections are motivated by our wish to find a characterization of perfect state transfer on translation graphs.

[1]Cayley graphs for abelian groups.

5.1 Cubelike graphs

Definition. Given a group G and a subset $\mathcal{C}$ closed under taking the inverse operation, the (undirected) *Cayley Graph* $\mathrm{Cay}(G, \mathcal{C})$ is the graph whose vertices are the elements of G, and two distinct vertices are adjacent if and only if their group difference is contained in $\mathcal{C}$. The subset $\mathcal{C}$ is called the *connection set* of the Cayley Graph.

Definition. A graph X is called a *cubelike graph* if X is a Cayley Graph for the group $\mathbb{Z}_2^d$.

Definition. A *(multiplicative complex) character* χ of a group G is a homomorphism from G to the multiplicative group of complex numbers.

The set of all characters of a group forms the group $\mathrm{Hom}(G, \mathbb{C}^*)$. If G is finite, then the image of any character $\chi(G)$ lies in the unit circle, and in the case where $G = \mathbb{Z}_2^d$, we have that $\chi(g) = \pm 1$ for all characters χ and all $g \in G$.

If $X = \mathrm{Cay}(G, \mathcal{C})$ is a Cayley Graph for a finite abelian group G and χ is a character, let $\chi(\mathcal{C}) = \sum_{g \in \mathcal{C}} \chi(g)$, and note that we can see χ as a vector $\boldsymbol{\chi} \in \mathbb{C}^{|G|}$. Then

$$A(X)\ \boldsymbol{\chi} = \chi(\mathcal{C})\ \boldsymbol{\chi}.$$

It is not difficult to see that every cyclic group is isomorphic to its group of characters, and because every finite abelian group is isomorphic to a direct sum of cyclic groups, it follows that finite abelian groups of order n are isomorphic to their character groups. In particular, there are precisely n distinct characters, and each one of them is an eigenvector for $A(X)$. It is well known that the set of n characters of a finite abelian group G of order n is linearly independent, and so they are precisely the eigenvectors of $A(X)$ for any Cayley Graph X on G.

We can express the characters of $\mathbb{Z}_2^d$ explicitly by fixing $a \in \mathbb{Z}_2^d$ and setting, for all $x \in \mathbb{Z}_2^d$,

$$\chi_a(x) = (-1)^{a^T x}.$$

We now assume henceforth that $G = \mathbb{Z}_2^d$, and $\mathcal{C} \subset G$. Our goal is to determine when $X = \mathrm{Cay}(G, \mathcal{C})$ admits perfect state transfer, preferably in terms of a simple description of $\mathcal{C}$. Note that X is connected if and only if $\mathcal{C}$ generates G, a situation that we assume hereupon. Due to the structure of G, that is equivalent to $\mathcal{C}$ containing a basis for G seen as a vector space over $\mathbb{Z}_2$. Moreover, $\mathcal{C}$ is a basis if and only if X is isomorphic to the d-dimensional cube. So the maximum diameter of X is d, and the number of distinct eigenvalues is at least equal to $d+1$.

Godsil et al. [9] and Godsil and Cheung [18] have studied perfect state transfer in cubelike graphs. We summarize below part of their findings.

5.1.1 Theorem (Godsil and Cheung [18], Theorem 2.3)**.** *Suppose* $X = \mathrm{Cay}(\mathbb{Z}_2^d, \mathcal{C})$. *Let* $w = \sum_{g \in \mathcal{C}} g$. *Let* $P_w = A(\mathrm{Cay}(\mathbb{Z}_2^d, \{w\})$. *Then*

$$U_A\left(\frac{\pi}{2}\right) = \mathtt{i}^{|\mathcal{C}|} P_w.$$

5.1.2 Corollary. *Suppose* $X = \mathrm{Cay}(\mathbb{Z}_2^d, \mathcal{C})$. *Let* $w = \sum_{g \in \mathcal{C}} g$. *If* $w \neq 0$, *then* X *admits perfect state transfer between vertices* u *and* $u + w$ *at time* $\frac{\pi}{2}$ *for all* $u \in V(X)$.

When $\sum_{g \in \mathcal{C}} g = 0$, the situation is more delicate. The connection set of any cubelike graph determines a matrix M whose columns are the vectors in the connection set $\mathcal{C}$. A matrix M whose columns are vectors over $\mathbb{Z}_2$ determines a binary linear code, which we will refer to as C. Its *codewords* are the vectors in the row-space of M. The *weight* of a codeword $c \in C$ is the number of entries which are not zero, and is denoted by $\mathrm{wt}(c)$.

Let $\widetilde{M}$ be the lift of the matrix M to $\mathbb{Z}$. Let Δ be the gcd of the entries of $\widetilde{M}\mathbf{j}$, or equivalently the gcd of the weights of the rows of M. We say that the *centre* of C is the projection onto $\mathbb{Z}_2$ of the vector $\dfrac{1}{\Delta}\widetilde{M}\mathbf{j}$.

The following result generalizes the theorem above, and deals with the case where $\sum_{g \in \mathcal{C}} g = 0$.

5.1.3 Theorem (Godsil and Cheung [18], Theorem 4.1 and Corollary 4.2)**.** *Let* X *be a cubelike graph in* $\mathbb{Z}_2^d$ *with associated matrix* M *and code* C. *Let* Δ *be the gcd of the weights of the rows of* M. *The following are equivalent.*

(i) *There is some* $w \in \mathbb{Z}_2^d$ *such that perfect state transfer occurs from* u *to* $u + w$ *at time* $\frac{\pi}{2\Delta}$ *for all* $u \in V(X)$.

(ii) All codewords of C have weight divisible by Δ, and, for all $a \in \mathbb{Z}_2^d$, there is a $w \in \mathbb{Z}_2^d$ such that

$$\frac{1}{\Delta}\operatorname{wt}(a^T M) \equiv a^T w \pmod 2.$$

(iii) Δ divides $|\operatorname{supp}(a) \cap \operatorname{supp}(b)|$ for any two codewords a and b.

If any of the cases hold, then w must be the centre of the code.

The theorem above presents a characterization of perfect state transfer in cubelike graphs. However, to check whether a cubelike graph $(\mathbb{Z}_2^d, \mathcal{C})$ with $\sum_{g\in\mathcal{C}} g = 0$ admits perfect state transfer one needs to examine all codewords of the code associated to the graph. We also cannot use the theorem to construct cubelike graphs admitting perfect state transfer at arbitrarily small times, despite the existence of these examples as observed by Chan in [17].

We would like to accomplish some success in either of the problems mentioned above. In the direction of the first problem, we present the preliminary results below.

Definition. A complex matrix M is called *flat* if the absolute value of each of its entries is constant.

Definition. We say that a graph X with adjacency matrix A admits *(instantaneous) uniform mixing* at time τ if $U_A(\tau)$ is a flat complex matrix.

The study of uniform mixing has been the topic of a good number of recent papers, see for instance [60], [32], [1], [2], [16], and [41]. In the context of cubelike graphs, it was studied by Chan in [17]. Here we will show that uniform mixing in cubelike graphs is intimately related to perfect state transfer.

Because non-singular linear endomorphisms of $\mathbb{Z}_2^n$ are automorphisms of the graph, every (connected) cubelike graph is isomorphic to a cubelike graph whose set of generators contains the standard basis of $\mathbb{Z}_2^d$, which we denote by $\beta = \{\mathbf{f}_1, ..., \mathbf{f}_d\}$. We say that these graphs are in *standard form*.

5.1.4 Theorem. *Let $X = \operatorname{Cay}(\mathbb{Z}_2^d, \mathcal{C})$ be a cubelike graph in standard form, that is, $\mathcal{C} = \beta \cup \mathcal{C}'$. If X admits perfect state transfer and $\sum_{g\in\mathcal{C}} g = 0$, then the following conditions hold.*

(a) $X' = \mathrm{Cay}(\mathbb{Z}_2^d, \mathcal{C}')$ *admits uniform mixing at time* $\frac{\pi}{4}$.

(b) $|\mathcal{C}'| \geq d$.

Proof. Let B be the adjacency matrix of $\mathrm{Cay}(\mathbb{Z}_2^d, \beta)$ and C be that of $\mathrm{Cay}(\mathbb{Z}_2^d, \mathcal{C}')$. Note that $A(X) = B + C$, and B and C are commuting matrices. Hence

$$U_A(t) = U_B(t)U_C(t), \quad \text{and so} \quad U_C(t) = U_A(t)\overline{U_B(t)}.$$

From Theorem 5.1.1, it follows that if perfect state transfer happens in X, it must be at time $\frac{\pi}{4}$ or smaller. Hence $U_A\left(\frac{\pi}{4}\right)$ is a multiple of a permutation matrix which either is the identity or has order two and no fixed points. On the other hand, $U_B\left(\frac{\pi}{4}\right)$ is a flat complex matrix. Thus $U_C\left(\frac{\pi}{4}\right)$ is flat. If X' were disconnected, then $U_C(t)$ would be a diagonal block matrix with at least two blocks. As a consequence the graph X' is connected, so $|\mathcal{C}'| \geq d$. □

We finish this section with an application of the method we developed in Chapter 4. Recall that we denote $P_w = A(\mathrm{Cay}(\mathbb{Z}_2^d, \{w\})$.

5.1.5 Theorem. *Let* $X = \mathrm{Cay}(\mathbb{Z}_2^d, \mathcal{C})$, $A = A(X)$. *Let* $\mathcal{C}' \subset \mathcal{C}$ *be the set containing the elements of* $\mathcal{C}$ *which are non-zero in the* i*-th entry, with* $1 \leq i \leq d$. *Let* C *be the adjacency matrix of* $\mathrm{Cay}(\mathbb{Z}_2^d, \mathcal{C}')$. *Suppose also that* $\sum_{g \in \mathcal{C}} g = 0$. *Suppose finally that* X *admits perfect state transfer at time* $\tau = \frac{\pi}{2^\alpha}$ *with* $\alpha > 1$, *and so* $U_A(\tau)$ *is a multiple of* P_w *for some* w. *Then*

a) $U_C(2\tau) = (-1)^{\langle e_i, w\rangle} I$.

b) $\sum_{g \in \mathcal{C}'} g = 0$.

c) *If* $\alpha > 2$, *then* $|\mathcal{C}'| \equiv 0 \pmod 4$.

d) *If* $\alpha = 2$, *then* $|\mathcal{C}'| \equiv 0 \pmod 4$ *if* $\langle \boldsymbol{e}_i, w\rangle = 0$, *and* $\equiv 2 \pmod 4$ *if* $\langle \boldsymbol{e}_i, w\rangle = 1$.

Proof. Suppose without loss of generality that $i = 1$. Then, for some matrix B,

$$A = \mathtt{I}_2 \otimes B + A(K_2) \otimes C.$$

As a consequence, if $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$,

$$(H \otimes \mathtt{I})A(X)(H \otimes \mathtt{I}) = \begin{pmatrix} B+C & 0 \\ 0 & B-C \end{pmatrix},$$

and so we have

$$(H \otimes \mathtt{I})U_A(H \otimes \mathtt{I}) = \begin{pmatrix} U_B U_C & 0 \\ 0 & U_B U_C^{-1} \end{pmatrix}.$$

By hypothesis, $U_A(\tau) = P_w$, and so

$$(H \otimes \mathtt{I})P_w = \begin{pmatrix} U_B(\tau)U_C(\tau) & 0 \\ 0 & U_B(\tau)U_C(\tau)^{-1} \end{pmatrix}(H \otimes \mathtt{I}).$$

If $\langle \mathbf{e}_1, w \rangle = 0$, this is equivalent to

$$P_w = \begin{pmatrix} U_B(\tau)U_C(\tau) & 0 \\ 0 & U_B(\tau)U_C(\tau)^{-1} \end{pmatrix} \quad \text{and}$$

$$P_{w+\mathbf{e}_1} = \begin{pmatrix} 0 & U_B(\tau)U_C(\tau) \\ U_B(\tau)U_C(\tau)^{-1} & 0 \end{pmatrix},$$

and so $U_C(\tau) = U_C(\tau)^{-1}$, implying that $U_C(2\tau) = \mathtt{I}$. Otherwise $\langle \mathbf{e}_1, w \rangle = 1$, and we have

$$P_w = \begin{pmatrix} 0 & U_B(\tau)U_C(\tau) \\ -U_B(\tau)U_C(\tau)^{-1} & 0 \end{pmatrix} \quad \text{and}$$

$$P_{w+\mathbf{e}_1} = \begin{pmatrix} U_B(\tau)U_C(\tau) & 0 \\ 0 & -U_B(\tau)U_C(\tau)^{-1} \end{pmatrix},$$

thus $U_C(\tau) = -U_C(\tau)^{-1}$, and $U_C(2\tau) = -\mathtt{I}$.

In any case, $U_C\left(\frac{\pi}{2}\right)$ is a multiple of the identity. In view of Theorem 5.1.1, $U_C\left(\frac{\pi}{2}\right) = \mathtt{i}^{|\mathcal{C}'|}P_q$ where $q = \sum_{g \in \mathcal{C}'} g$. Because $P_q = \mathtt{I}$, then $q = 0$. Thus $|\mathcal{C}'| \equiv 0 \pmod 4$, unless $2\tau = \frac{\pi}{2}$ and $\langle \mathbf{e}_1, w \rangle = 1$, in which case $|\mathcal{C}'| \equiv 2 \pmod 4$. $\square$

5.2 Circulant graphs

In this short section, we comment on the problem of characterizing perfect state transfer in another class of Cayley graphs.

Definition. A graph X is called a *circulant graph* if it is a Cayley graph for $\mathbb{Z}_n$ for some $n \in \mathbb{N}$.

In a sequence of papers ([7], [62], [8]), Bašić and others fully characterized when circulant graphs admit perfect state transfer. We introduce some notation. Let

$$G_n(d) = \{k : \gcd(k, n) = d\}.$$

The following result is a corollary of a more general result due to Bridges and Mena [12, Theorem 2.4].

5.2.1 Theorem. *A circulant graph for $\mathbb{Z}_n$ with connection set $\mathcal{C}$ has an integral spectrum if and only if, for some set D of proper divisors of n,*

$$\mathcal{C} = \bigcup_{d \in D} G_n(d).$$

Given a set D of proper divisors of n, we define

$$D_i = \{d \in D : \left|\frac{n}{d}\right|_2 = 2^{-i}\}.$$

We also denote $D_i^* = D_i \backslash \left\{\frac{n}{2^i}\right\}$.

5.2.2 Theorem (Bašić [8], Theorem 22). *A (connected) circulant graph $X = \mathrm{Cay}(\mathbb{Z}_n, \mathcal{C})$ on more than 2 vertices admits perfect state transfer if and only if all of the following conditions hold.*

(i) X has integral spectrum, and so there is a subset D of proper divisors of n such that $\mathcal{C} = \bigcup_{d \in D} G_n(d)$.

(ii) n is a multiple of 4.

(iii) Either $\frac{n}{2}$ or $\frac{n}{4}$ belongs to $\mathcal{C}$, but not both.

(iv) $2D_2^* = D_1^*$.

(v) $4D_2^* = D_0$.

The proof available for the result above is split into several steps and relies on some theory about Ramanujan's sums. We would like to see a more direct proof of the result. It is also neither stated in the paper nor explicit in the original proof at which time perfect state transfer occurs. For that, we offer the contribution below.

Let ω_n denote a primitive n-th root of unity, and define for all $j \in \{0, ..., (n-1)\}$,

$$\mathbf{v}_j = (1\ \omega_n^j\ \omega_n^{2j}\ \ldots\ \omega_n^{(n-1)j}).$$

For any circulant graph on $\mathbb{Z}_n$ with connection set $\mathcal{C}$, the set $\{\mathbf{v}_0, ..., \mathbf{v}_{n-1}\}$ is a basis of orthogonal eigenvectors, and the eigenvalue corresponding to $\mathbf{v}_j$ is

$$\lambda_j = \sum_{g\in\mathcal{C}} \omega_n^{sj}.$$

We also denote $\mathcal{C}_a = \left\{g \in \mathcal{C} : |g|_2 = \frac{1}{2^a}\right\}$, and $\mathcal{C}_{\geq a} = \left\{g \in \mathcal{C} : |g|_2 \leq \frac{1}{2^a}\right\}$.

5.2.3 Lemma. *Let $n = 2^e f$. Then for any $q \in \{1, ..., e\}$,*

$$\lambda_{\frac{n}{2^q}} = |\mathcal{C}_{\geq q}| - |\mathcal{C}_{q-1}|,$$

and consequently

$$\lambda_0 - \lambda_f = \sum_{a=0}^{e-2} |\mathcal{C}_a| + 2|\mathcal{C}_{e-1}|.$$

Proof. First note that

$$\lambda_{\frac{n}{2^q}} = \sum_{g\in\mathcal{C}} \omega_{2^q}^g.$$

Suppose $e = 1$. Note that $\omega_2^g = (-1)^g$ (seeing $g \in \mathbb{Z}$), and so

$$\lambda_{\frac{n}{2}} = |\mathcal{C}_{\geq 1}| - |\mathcal{C}_0|,$$

hence

$$\lambda_0 - \lambda_{\frac{n}{2}} = 2|\mathcal{C}_0|.$$

Suppose $e > 1$. Suppose $g \in \mathcal{C}$, and the power of 2 dividing g is smaller than $q-1$. Let $g' = \frac{n}{2^{e-q+1}} + g$. Then

$$\gcd(g, g') = g,$$

and so because the graph has integer eigenvalues, it follows that $g' \in \mathcal{C}$. Note that

$$\omega_n^{g2^{e-q}f} = -\omega_n^{g'2^{e-q}f},$$

thus

$$\sum_{g \in \mathcal{C}} \omega_n^{g\frac{n}{2^q}} = |\mathcal{C}_{\geq q}| - |\mathcal{C}_{q-1}|.$$

□

We believe the following theorem might be a first step towards an elementary proof of Theorem 5.2.2, but its importance at this point is that it determines at which time perfect state transfer happens in circulant graphs.

5.2.4 Theorem. *Suppose $n = 2^e f$, with $e \geq 2$. Suppose perfect state transfer happens in X at time τ. Then $\tau = \frac{\pi}{2}$ if and only if $\frac{n}{4} \in \mathcal{C}$ and $\frac{n}{2} \notin \mathcal{C}$, or $\frac{n}{4} \notin \mathcal{C}$ and $\frac{n}{2} \in \mathcal{C}$. Using Theorem 5.2.2, this means that perfect state transfer in circulants always happens at time $\tau = \frac{\pi}{2}$.*

Proof. Let $g \in \mathcal{C}$ be such that the power of 2 in the factorization of g is smaller than $e-1$. It follows that for $g' \in \left\{\frac{n}{2} - g,\ \frac{n}{2} + g,\ n - g\right\}$,

$$\gcd(g, g') = g.$$

Because the eigenvalues are integers, $\left\{\frac{n}{2} - g,\ \frac{n}{2} + g,\ n - g\right\} \subset \mathcal{C}$. Hence $|\mathcal{C}_a| \equiv 0 \pmod 4$ for all $a \leq e-2$. From Lemma 5.2.3, it follows that $|\{\frac{n}{2}, \frac{n}{4}\} \cap \mathcal{C}| = 1$ if and only if

$$\lambda_0 - \lambda_f \equiv 2 \pmod 4,$$

but from Theorem 2.4.4, this is equivalent to $\tau = \frac{\pi}{2}$. □

Chapter 6

Orthogonal polynomials and spectrally extremal graphs

In this chapter, we study the relation between certain orthogonal polynomials and perfect state transfer. First, we introduce an inner product in the space of polynomials that depends on the adjacency matrix of the graph. These polynomials evaluated on the adjacency matrix of the graph yield an orthogonal basis of matrices. We will cover basic properties of these polynomials and matrices. Even though this is a well established theory, we offer an original observation in Corollary 6.1.3.

Following this, we relate the orthogonal basis of matrices to the distance matrices of the graph. In the case where the graph is distance-regular, these matrices coincide, but in general they are very different. However, if the graph is extremal with respect to the known bound on the number of eigenvalues given by the diameter plus one, then the work of Fiol, Garriga and others provides a vast literature about the relation between orthogonal polynomials and distance matrices (see for instance [29], [24], [57] and [65]).

Finally, we relate all these concepts to perfect state transfer. More specifically, we show how we can find strongly cospectral vertices in certain cases, and then show which conditions on the parity of the eigenvalues are needed to attain perfect state transfer. The relation between graphs of diameter d with $d+1$ eigenvalues and perfect state transfer is considered in Bu et al. [68]. Our approach is nevertheless more general and with deeper consequences. In this section we will also provide an elementary proof of Lemma 3.2.2.

6.1 Orthogonal polynomials and matrices

We refer to Godsil [36, Chapter 8] for most of the results in this section.

Let $\mathcal{P}_d$ be the vector space of polynomials with real coefficients and degree at most d.

6.1.1 Theorem. *If $\langle\ ,\ \rangle$ is an inner product of $\mathcal{P}_d$ satisfying $\langle xp(x), q(x)\rangle = \langle p(x), xq(x)\rangle$ for all p and q, and if $p_0, p_1, ..., p_d$ is a sequence of orthogonal polynomials obtained after applying the Gram-Schmidt algorithm to $x^0, x^1, ..., x^d$, then the following holds.*

(i) *p_r is the unique polynomial up to multiplication by scalar which is orthogonal to p_0, p_1,...,p_{r-1}.*

(ii) *There are coefficients $\{a_r, b_r, c_r\}_{r=0}^{d}$ such that, for all $r \in \{0, ..., d\}$,*

$$xp_r(x) = c_{r+1}p_{r+1}(x) + a_r p_r(x) + b_{r-1}p_{r-1}(x), \tag{6.1}$$

with the conventions that $b_{-1} = c_{d+1} = 0$.

(iii) *The zeros of each polynomial are real and simple. Moreover, the zeros of p_r interlace those of p_{r+1} for all r.*

Proof. Item (i) is a simple consequence of a dimension argument. For (ii), note that, for all r, the polynomial $xp_{r-2}(x)$ is a linear combination of polynomials with degree at most $r-1$, and hence

$$\langle xp_r(x), p_{r-2}(x)\rangle = \langle p_r(x), xp_{r-2}(x)\rangle = 0.$$

Hence $xp_r(x)$ is a linear combination of p_{r+1}, p_r and p_{r-1} for all r.

For (iii), suppose without loss of generality that the leading coefficient of all polynomials is positive, and so $c_r > 0$ for all r. Note that (ii) implies that

$$b_{r-1} = \frac{c_r\langle p_r, p_r\rangle}{\langle p_{r-1}, p_{r-1}\rangle},$$

and so $b_r > 0$ for all r. Now, $\left(\frac{p_0}{p_1}\right)' < 0$ for all x (including the value $-\infty$ at certain limits where it is not defined). Suppose that $\left(\dfrac{p_{r-1}}{p_r}\right)' < 0$. Reorganizing Equation 6.1, we get

$$c_{r+1}\frac{p_{r+1}(x)}{p_r(x)} = x - a_r - b_{r-1}\frac{p_{r-1}(x)}{p_r(x)},$$

and so by induction, for all r, we have $\left(\dfrac{p_r}{p_{r+1}}\right)' < 0$. As a consequence,

$$p_r' p_{r+1} - p_r p_{r+1}' < 0. \tag{6.2}$$

Suppose by induction that all zeros of p_r are all real and simple. So the derivative of p_r changes signs between any two of its consecutive zeros, thus Equation 6.2 implies that p_{r+1} has an odd number of real zeros between them. Moreover, these polynomials have positive leading coefficients, so p_{r+1} is negative at the largest zero of p_r, thus it must have a zero which is larger than the zeros of p_r, and likewise, a zero which is smaller. As a consequence, all zeros of p_{r+1} are real, simple, and are interlaced by those of p_r. $\square$

There are many inner products of polynomials, but here we focus on a seemingly boring case. In the vector space of square matrices with complex entries, the product

$$\langle A, B\rangle = \operatorname{tr}(AB^*)$$

is an inner product, which we will refer to as the *trace product*, and so we have the following definition.

Definition. Given a symmetric matrix A whose minimal polynomial has degree $d+1$, we define an inner product $\langle\ ,\ \rangle_A$ in the space of polynomials of degree at most d by

$$\langle p(x), q(x)\rangle_A = \operatorname{tr}(p(A)q(A)).$$

We will omit the subscript A whenever it is determined by the context.

Given a symmetric matrix A whose minimal polynomial has degree $d+1$, and according to the inner product defined above, we can obtain a sequence of orthogonal polynomials

$(p_0, ..., p_d)$ of increasing degree by applying the Gram-Schmidt procedure to $(x^0, ..., x^d)$. Note in particular that $p_1(x) = \alpha x$ for some constant α.

As a consequence, the vector space $\langle \{A^k\}_{k \geq 0} \rangle$ admits two very distinct orthogonal bases of matrices with respect to the trace product. One is formed by the orthogonal projections onto the eigenspaces of A. They satisfy $E_r E_s = \mathtt{0}$ if $r \neq s$, and so trivially

$$\operatorname{tr}(E_r E_s) = 0.$$

The other basis is $\{p_0(A), ..., p_d(A)\}$, which is an orthogonal basis by definition of the polynomials. These two bases are very different. For example, each projector E_r is a polynomial of degree d evaluated at A.

We finish this section with a useful observation. It is a generalization of the Koppinen identity for the Bose-Mesner algebra of an association scheme (see [56]).

6.1.2 Theorem. *Let $\mathcal{A}$ be a vector space of square matrices of order n with complex entries, and let $\{A_0, ..., A_d\}$ and $\{B_0, ..., B_d\}$ be two orthogonal bases with respect to the trace product. Then*

$$\sum_{r=0}^{d} \frac{1}{\operatorname{tr}(A_r A_r^*)} A_r \otimes A_r^* = \sum_{r=0}^{d} \frac{1}{\operatorname{tr}(B_r B_r^*)} B_r \otimes B_r^*.$$

Proof. Consider the canonical isomorphism $\varphi : \mathbb{C}^{n \times n} \to \mathbb{C}^{n^2}$ that maps the matrix which is 1 at the position (i, j) and 0 elsewhere to the vector $\mathbf{e}_{i+(j-1)n}$. Note that

$$\operatorname{tr}(AB^*) = \varphi(B)^* \varphi(A),$$

and so $\{\varphi(A_0), ..., \varphi(A_d)\}$ and $\{\varphi(B_0), ..., \varphi(B_d)\}$ are orthogonal bases of $\varphi(\mathcal{A})$ with respect to the canonical inner product. For any orthogonal basis $\{\mathbf{v}_0, ..., \mathbf{v}_d\}$ of $\varphi(\mathcal{A})$, the known formula for the orthogonal projection onto $\varphi(\mathcal{A})$ is

$$\operatorname{proj}_{\varphi(\mathcal{A})} = \sum_{r=0}^{d} \frac{1}{\mathbf{v}_r^* \mathbf{v}_r} \mathbf{v}_r \mathbf{v}_r^*,$$

and hence

$$\sum_{r=0}^{d} \frac{1}{\varphi(A_r)^* \varphi(A_r)} \varphi(A_r) \varphi(A_r)^* = \sum_{r=0}^{d} \frac{1}{\varphi(B_r)^* \varphi(B_r)} \varphi(B_r) \varphi(B_r)^*.$$

A simple reorganization of the terms on these $n^2 \times n^2$ matrices yields the result. $\square$

Recall that if E is an orthogonal projection onto a subspace S, then

$$\operatorname{tr} E = \dim S.$$

If X is a graph with distinct eigenvalues $\{\theta_0, ..., \theta_d\}$, we typically denote the multiplicity of θ_r by m_r.

6.1.3 Corollary. *Let X be a graph and $\{E_0, ..., E_d\}$ be the orthogonal projections onto the eigenspaces of $A = A(X)$. Let $(p_0(x), ..., p_d(x))$ be a sequence of polynomials of increasing degree, orthogonal with respect to trace product. Then*

$$\sum_{r=0}^{d} \frac{1}{m_r} E_r \otimes E_r = \sum_{r=0}^{d} \frac{1}{\operatorname{tr}(p_r(A)^2)} \; p_r(A) \otimes p_r(A).$$

$\square$

6.2 Distance matrices and equitable partitions

If X is a distance-regular graph of diameter d, then the distance matrices $\{A_0, A, A_2, ..., A_d\}$ form an association scheme, and it follows from the definition of the intersection array of X that (see Equation 3.2)

$$AA_i = b_{i-1} A_{i-1} + a_i A_i + c_{i+1} A_{i+1}.$$

As a consequence, the matrix A_i can be written as a polynomial of degree i on A, say p_i. Note that

$$\operatorname{tr}(A_i A_j) = \text{sum of all entries of } (A_i \circ A_j),$$

and hence the polynomials $(p_0, ..., p_d)$ form a sequence of polynomials of increasing degree satisfying $\operatorname{tr}(p_i(A) p_j(A)) = 0$ if $i \neq j$. They are the orthogonal polynomials obtained from applying Gram-Schmidt to the sequence $(x^0, ..., x^d)$. It turns out that distance-regular graphs are characterized by this property (see Fiol [28]).

We will now study the relation between orthogonal polynomials and distance-regularity through a local perspective.

Definition. Suppose $\pi = (C_1, ..., C_k)$ is a partition of $V(X)$. We say that π is an *equitable partition* if the number of edges from a vertex $u \in C_i$ to a cell C_j depends only on i and j, say $c(i, j)$. The numbers $c(i, j)$ are called the *parameters* of the partition.

6.2.1 Lemma (Godsil [36], Chapter 5, Lemma 3.1)**.** *If the distance partition relative to $u \in V(X)$ is equitable, the number of closed walks on u of any length depends only on the parameters of the partition.*

By induction on the length of a walk, we have the following corollary.

6.2.2 Lemma. *If the distance partitions of vertices u and v are equitable, and if u and v are cospectral vertices, then the parameters of their partitions are equal.*

It follows trivially from the definitions that a graph is distance-regular if and only if the distance partition relative to each vertex is equitable and the parameters do not depend on the chosen vertex. This can be strengthened by the following theorem.

6.2.3 Theorem (Godsil and Shawe-Taylor [43], Theorem 2.2)**.** *If X is regular and the distance partition relative to each vertex is equitable, then X is distance-regular.*

We introduce some definitions below.

Definition. Given a vertex $u \in V(X)$, the maximum distance between u and any vertex of X is called the *eccentricity* of u and will be denoted by ε_u. We also define the *dual degree* of u as $\mathrm{d}^*_u = |\Phi_u| - 1$. Finally, the *walk module* of u is the subspace

$$W_u = \langle \{A^k \mathbf{e}_u\}_{k \geq 0} \rangle.$$

It follows that

$$W_u = \langle \{E_r \mathbf{e}_u\}_{\theta_r \in \Phi_u} \rangle,$$

and because the vectors $\{A^k \mathbf{e}_u\}_{k=0}^{\varepsilon_u}$ are all independent, we have that

$$\varepsilon_u \leq \mathrm{d}^*_u. \tag{6.3}$$

If equality is met above, we say that u is a *spectrally extremal* vertex.

Definition. Let X be a graph, $A = A(X)$, and $u \in V(X)$. We define the u-th *local inner product* in the space of polynomials of degree at most d_u^* by

$$\langle p, q\rangle_u = \mathbf{e}_u^T p(A) q(A) \mathbf{e}_u.$$

In terms of this inner product, equitable distance partitions can be characterized as follows.

6.2.4 Proposition. *Let $(p_0, ..., p_{\mathrm{d}^*})$ be a sequence of orthogonal polynomials of increasing degree with respect to the u-th local inner product. The distance partition relative to u is equitable if and only if $p_r(A)\boldsymbol{e}_u$ is a 01-vector (up to scalar) whose support consists precisely of the vertices at distance r from u. In particular, u is spectrally extremal.*

Proof. The key property of orthogonal polynomials useful for this proposition is the three term recurrence (Equation 6.1) from Theorem 6.1.1

$$Ap_r(A)\mathbf{e}_u = c_{r+1}p_{r+1}(A)\mathbf{e}_u + a_r p_r(A)\mathbf{e}_u + b_{r-1}p_{r-1}(A)\mathbf{e}_u.$$

If the extra hypothesis on the polynomials is true, the equation above says precisely that the number of neighbours in $p_r(A)\mathbf{e}_u$ of any vertex in each of the sets $p_{r+1}(A)\mathbf{e}_u$, $p_r(A)\mathbf{e}_u$ and $p_{r-1}(A)\mathbf{e}_u$ does not depend on the choice of the vertex. Thus the distance partition relative to u is equitable.

Conversely, start by noting that $p_0(A) = \mathtt{I}$ and $p_1(A) = A$. Now suppose by induction that for all $k \leq r$, the vector $p_k(A)\mathbf{e}_u$ is a 01-vector whose support consists precisely of the vertices at distance k from u. Because the distance partition of u is equitable, $Ap_r(A)\mathbf{e}_u$ is constant on the vertices at a fixed distance from u, and its support is confined to vertices at distance $(r-1)$, r and $(r+1)$ from u. By induction, orthogonality, and the three term recurrence, $p_{r+1}(A)\mathbf{e}_u$ is a vector constant on the vertices at distance $r+1$ from u, and 0 elsewhere. □

For regular graphs, this result can be significantly strengthened.

6.2.5 Theorem (Fiol, Garriga and Yebra [30], Theorem 6.3)**.** *If the distance partition relative to a vertex u is equitable, then u is spectrally extremal and there exists a polynomial $p(x)$ such that $p(A)\boldsymbol{e}_u$ is a 01-vector whose support are the vertices at distance d_u^* from u. If the graph is regular, then the converse holds.*

6.3 Spectrally extremal vertices and quantum walks

In this section, we focus on the case where a graph contains spectrally extremal vertices, and we study when such vertices can be involved in perfect state transfer. More specifically, we find a characterization of strong cospectrality between spectrally extremal vertices.

6.3.1 Lemma. *Let $u, v \in V(X)$, with $g = d(u,v)$. Suppose u is a spectrally extremal vertex. If u and v are strongly cospectral, then the following conditions hold.*

(i) If $d(u,w) = d(u,v)$, then $w = v$.

(ii) If $z \in V(X)$, if $\Phi_z = \Phi_u$ and if $d(z,w) = d(u,v)$ for some $w \in V(X)$, then $(A^g)_{z,w} \leq (A^g)_{u,v}$. Equality occurs if and only if z and w are also strongly cospectral.

Proof. Suppose $\Phi_u = \{\theta_0, \theta_1, ..., \theta_{\mathrm{d}^*}\}$. For all $r \in \{0, ..., \mathrm{d}^*\}$, let $\sigma_r \in \{+1, -1\}$ be such that

$$E_r \mathbf{e}_v = \sigma_r E_r \mathbf{e}_u.$$

Let $p(x)$ be the polynomial of minimum degree satisfying $p(\theta_r) = \sigma_r$ for all r. Then it follows that

$$p(A)\mathbf{e}_u = \mathbf{e}_v.$$

Because $\varepsilon_u = \mathrm{d}^*$, the vector $p(A)\mathbf{e}_u$ must be non-zero on the entries corresponding to vertices whose distance to u is the degree of $p(x)$. Hence deg $p(x) = g$, and v is the unique vertex at distance g from u.

To see (ii), first note that $\langle p(A)\mathbf{e}_z, p(A)\mathbf{e}_z \rangle = 1$, so the absolute value of each entry in $p(A)\mathbf{e}_z$ is at most 1. Let $p(x) = a_g x^g + ... + a_0$. Then $p(A)\mathbf{e}_u = \mathbf{e}_v$ implies that

$$a_g = \frac{1}{(A^g)_{u,v}},$$

and thus

$$1 \geq |p(A)_{z,w}| = a_g (A^g)_{z,w} = \frac{(A^g)_{z,w}}{(A^g)_{u,v}}.$$

□

6.3.2 Lemma. *Let $u, v \in V(X)$. The following are equivalent.*

(i) Vertices u and v are cospectral, and there exists a polynomial $p(x)$ such that $p(A)\boldsymbol{e}_u = \boldsymbol{e}_v$.

(ii) The vertices u and v are strongly cospectral.

Moreover, if u and v are cospectral, then any polynomial satisfying $p(A)\boldsymbol{e}_u = \boldsymbol{e}_v$ is such that $p(A)\boldsymbol{e}_v = \boldsymbol{e}_u$ and $p(\theta_r) = \pm 1$ for all $\theta_r \in \Phi_u$.

Proof. The implication (ii) $\implies$ (i) is trivial. To see the converse, let $p(x)$ be a polynomial satisfying $p(A)\mathbf{e}_u = \mathbf{e}_v$. Because $p(A)$ is a symmetric matrix, it follows that $(p(A)^2)_{u,u} = 1$. Vertices u and v are cospectral, so Theorem 2.5.1 implies that $(p(A)^2)_{v,v} = 1$. Thus $p(A)\mathbf{e}_v$ is a unitary vector, but $p(A)_{u,v} = 1$, implying that $p(A)\mathbf{e}_v = \mathbf{e}_u$. As a consequence, $p(A)^2\mathbf{e}_u = \mathbf{e}_u$, and so if $\theta_r \in \Phi_u$, it follows that $p(\theta_r) = \pm 1$. This shows that u and v are strongly cospectral. □

Here we introduce a definition. We say that u and v are (a pair of) *antipodal vertices* if the distance partition of u is equitable, $\{v\}$ is a singleton in the partition at maximum distance from u, and the parameters of the partition are symmetric with respect to u and v. Our use of the word "antipodal" here is consistent with its use in Chapter 3, in particular note that an antipodal distance-regular graph with classes of size 2 is partitioned into pairs of antipodal vertices.

6.3.3 Theorem. *If u and v are antipodal vertices in X, then u and v are spectrally extremal vertices and they are strongly cospectral. If X is regular, u is spectrally extremal , u and v are strongly cospectral, and their distance is equal to their eccentricity, then u and v are antipodal vertices.*

Proof. If u and v are antipodal, then the weaker direction of Theorem 6.2.5 implies that u is spectrally extremal and that there is a polynomial $p(x)$ such that

$$p(A)\mathbf{e}_u = \mathbf{e}_v.$$

From Lemma 6.3.2, we have that u and v are strongly cospectral.

For the converse, note that it follows from Theorem 6.2.5 that the distance partitions of u and of v are equitable. To see that the parameters of the partitions are symmetric with respect to u and v, note that if the vertices are strongly cospectral, then they are cospectral, and so by Lemma 6.2.2 the vertices u and v are antipodal. $\square$

We would like to drop the condition on the theorem above that requires u and v to be at maximal distance. In other words, we would like to believe that a pair of spectrally extremal strongly cospectral vertices in a regular graph must be at maximal distance from each other. For instance, this is true for 2-connected graphs. In particular, Lemma 6.3.1 implies that v is a cut-vertex of X, unless v is at maximal distance from u. If X is 2-connected, it follows that u and v must be at maximal distance.

For graphs which are not 2-connected, we were unable to achieve success in removing the hypothesis. The following lemma is a step towards this goal, but otherwise our failed efforts only indicate that it might not be possible. The consequences we derive from the lemma are nevertheless important.

6.3.4 Lemma. *Suppose u is a spectrally extremal vertex of X, and suppose u and v are strongly cospectral. Let $p(x)$ be the polynomial satisfying $p(A)\boldsymbol{e}_u = \boldsymbol{e}_v$, with $p(\theta_r) = \sigma_r \in \{+1, -1\}$ for all $\theta_r \in \Phi_u$. Let X' be the component of $X \backslash v$ containing u. Then $p(x)$ is the minimal polynomial with respect to u in X' (up to a constant).*

Proof. Let $d(u, v) = g$ and $A' = A(X')$. From Lemma 6.3.1 (i), we have that v is the unique vertex at distance g from u. Note that walks of length g pass by v only if v is its final vertex, so the entries of $p(A)\mathbf{e}_u$ relative to vertices at distance at most $g-1$ from u are equal to the respective entries of $p(A')\mathbf{e}_u$, thus $p(A')\mathbf{e}_u = 0$. Because the eccentricity of u in X' is $g-1$ and $p(x)$ has degree g, it follows that it is the minimal polynomial up to a constant. $\square$

6.3.5 Corollary. *Let $u, v \in V(X)$. Suppose $\Phi_u = \{\theta_0, ..., \theta_{\mathrm{d}^*}\}$, ordered in such a way that $\theta_r > \theta_{r+1}$ for all r. If u and v are spectrally extremal and strongly cospectral, and $p(x)$ is such that $p(A)\boldsymbol{e}_u = \boldsymbol{e}_v$, then there is no index $r \in \{0, ..., \mathrm{d}^*\}$ such that*

$$p(\theta_r) = p(\theta_{r+1}) = p(\theta_{r+2}).$$

Proof. Suppose otherwise that there is such index, say s. From Lemma 6.3.4, the roots of $p(x)$ are the eigenvalues of $X \backslash v$ in the support of u. A local version of interlacing implies that there are no two roots of $p(x)$ between θ_r and θ_{r+1} for any r, hence $p(\theta_s) = p(\theta_{s+1}) = p(\theta_{s+2})$ implies that there are three roots of the $p'(x)$ between two of its real roots. This is a contradiction to the fact that all roots of $p(x)$ are real. $\square$

If we know that the pair of strongly cospectral vertices is at maximal distance in a regular graph, we can actually determine the values of $p(\theta_r)$ for all r.

6.3.6 Theorem. *Let $u, v \in V(X)$. Suppose $\Phi_u = \{\theta_0, ..., \theta_{\mathrm{d}^*}\}$, ordered in such way that $\theta_r > \theta_{r+1}$ for all r. If u and v are antipodal then, for all $r \in \{0, ..., \mathrm{d}^*\}$,*

$$E_r \boldsymbol{e}_v = (-1)^r E_r \boldsymbol{e}_u.$$

If X is regular, then the converse holds.

Proof. Suppose X is regular. Let $d = d(u, v)$, and $p(x)$ the polynomial of degree d such that $p(A)\mathbf{e}_u = \mathbf{e}_v$. If $p(x)$ is such that $p(\theta_r) = (-1)^r$, then $p(x)$ has at least d^* roots, so $d \geq \mathrm{d}^*$, and hence it could only be that $d = \mathrm{d}^*$. So u and v are spectrally extremal, strongly cospectral, and at maximal distance. It follows from Theorem 6.3.3 that they are a pair of antipodal vertices.

Now suppose u and v are antipodal. A simple argument using Lemma 6.3.4 and interlacing will suffice to show this direction, but we provide an elementary proof below.

Let $p(x)$ be the polynomial satisfying $p(\theta_r) = \sigma_r \in \{+1, -1\}$ with $p(A)\mathbf{e}_u = \mathbf{e}_v$, and let $q(x)$ be the polynomial of minimal degree that satisfies $q(\theta_r) = (-1)^r$ for $r \in \{0, ..., \mathrm{d}^*\}$.

Our goal is to show that $\sigma_r = (-1)^r$. We have

$$\begin{aligned}
1 &\geq |q(A)_{u,v}| \\
&= \left| \sum_{r=0}^{\mathrm{d}^*} (-1)^r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s} \right| (A^{\mathrm{d}^*})_{u,v} \\
&= \left(\sum_{r=0}^{\mathrm{d}^*} (-1)^r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s} \right) (A^{\mathrm{d}^*})_{u,v}, \quad \text{because all terms are positive,} \\
&\geq \left(\sum_{r=0}^{\mathrm{d}^*} \sigma_r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s} \right) (A^{\mathrm{d}^*})_{u,v} \\
&= p(A)_{u,v} \\
&= 1.
\end{aligned}$$

Note that equality holds throughout if and only if $\sigma_r = (-1)^r$, as we wanted. □

If a graph X has diameter d, then Equation 6.3 implies that X has at least $d+1$ distinct eigenvalues. We say that X is *spectrally extremal* if equality holds. Note that every spectrally extremal graph contains at least one pair of spectrally extremal vertices.

6.3.7 Theorem. *Suppose X is a spectrally extremal regular graph on n vertices of diameter d, and that its distinct eigenvalues are $\theta_0 > \dots > \theta_d$. Suppose u and v are vertices at distance d. Then u and v are antipodal if and only if*

$$n \prod_{s=0}^{d} \frac{1}{\theta_0 - \theta_s} = \sum_{r=0}^{d} (-1)^r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s}.$$

Proof. Let $p(x)$ be a polynomial such that $p(A) = E_0$. Because the graph is regular $E_0 = (1/n)\mathtt{J}$, and so if $p(x) = a_d x^d + \dots + a_0$, it follows that, for all vertices u and v at distance d,

$$(A^d)_{u,v} = \frac{1}{n} \left(\prod_{s=0}^{d} \frac{1}{\theta_0 - \theta_s} \right)^{-1}.$$

The result now follows from Lemma 6.3.6. □

6.3.8 Corollary. *Suppose X is a spectrally extremal regular graph on n vertices of diameter d. If the eccentricity of every vertex is d and if*

$$n \prod_{s=0}^{d} \frac{1}{\theta_0 - \theta_s} = \sum_{r=0}^{d} (-1)^r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s},$$

then X is an antipodal distance regular graph.

Proof. It follows from Theorems 6.2.3 and 6.3.7. □

6.4 State transfer on spectrally extremal graphs

Now we apply our results to determine which spectrally extremal regular graphs admit perfect state transfer.

6.4.1 Theorem. *Suppose X is regular. Suppose u is a spectrally extremal vertex of X, and v is a vertex at maximal distance from u. Let $\Phi_u = \{\theta_0, ..., \theta_{\mathrm{d}^*}\}$, with $\theta_r > \theta_{r+1}$. Then X admits perfect state transfer between vertices u and v if and if only if the following conditions hold.*

(i) The eigenvalues in Φ_u are integers.

(ii) The vertices u and v are antipodal.

(iii) There is an α such that for all odd r, we have $|\theta_0 - \theta_r|_2 = 2^{-\alpha}$.

(iv) If r is even, then $|\theta_0 - \theta_r|_2 < 2^{-\alpha}$.

In that case, perfect state transfer happens at time $\frac{\pi}{2^\alpha}$ (or some odd multiple).

Proof. Theorem 2.4.3 implies that the eigenvalues are integers. From Theorem 2.4.2, perfect state transfer implies strong cospectrality. The vertices are at maximal distance from each other, and if they are strongly cospectral, Theorem 6.3.3 says that they are antipodal. Note that

$$U(t)\mathbf{e}_u = \sum_{r=0}^{\mathrm{d}^*} \mathsf{e}^{\mathtt{i}t\theta_r} E_r \mathbf{e}_u.$$

Lemma 6.3.6 implies that

$$\mathbf{e}_u = \sum_{r=0}^{\mathrm{d}^*} (-1)^r E_r \mathbf{e}_v,$$

therefore perfect state transfer is now equivalent to

$$\frac{\mathsf{e}^{\mathtt{i}t\theta_0}}{\mathsf{e}^{\mathtt{i}t\theta_r}} = (-1)^r,$$

and this is equivalent to

$$t(\theta_0 - \theta_r) = k_r \pi,$$

where k_r is an integer with the same parity as r. This condition is equivalent to (ii) and (iii), and also gives the expression for the time. □

In the case where X is spectrally extremal, we can say more.

6.4.2 Corollary. *Suppose X is a spectrally extremal regular graph of diameter d on n vertices, having distinct eigenvalues $\theta_0 > \ldots > \theta_d$. Then X admits perfect state transfer between any pair (u, v) of vertices at distance d if and only if*

(i) All eigenvalues are integers.

(ii) There is an α such that for all odd r, we have $|\theta_0 - \theta_r|_2 = 2^{-\alpha}$.

(iii) If r is even, then $|\theta_0 - \theta_r|_2 < 2^{-\alpha}$.

(iv) The following equality holds

$$n \prod_{s=0}^{d} \frac{1}{\theta_0 - \theta_s} = \sum_{r=0}^{d} (-1)^r \prod_{s \neq r} \frac{1}{\theta_r - \theta_s}.$$

Proof. It follows from Theorems 6.3.7 and 6.4.1. □

Using Theorem 6.3.7 again, we have the following corollary.

6.4.3 Corollary. *If X is a spectrally extremal regular graph of diameter d in which the eccentricity of every vertex is d, and if $U(\tau)$ is a permutation matrix with no fixed points for some τ, then X is a distance-regular graph.*

Chapter 7

Bipartite graphs, trees and the Laplacian matrix

This chapter is motivated by the question as to which trees admit perfect state transfer. We only have two examples of such trees: the paths P_2 and P_3. We realize that many of our observations generalize to bipartite graphs, and we find necessary conditions for the existence of perfect state transfer in such case. We were able for instance to show that trees whose adjacency matrix is invertible do not admit perfect state transfer. The problem remains open otherwise.

Following this, we introduce some properties of the Laplacian matrix of graphs, focusing on the Laplacian matrix of trees. We then approach for the first time in this thesis continuous-time quantum walk matrix relative to the Laplacian matrix of a graph. In this case, the problem is relatively easier, and we will show that eigenvalues in the support of vertices involved in perfect state transfer must be integers. As a consequence, many known results about the Laplacian spectrum of a graph can be applied to study perfect state transfer, and we will explore some of these relations.

7.1 Bipartite graphs

Suppose X is a bipartite graph, in which case the adjacency matrix of X can be written as

$$A(X) = \begin{pmatrix} \mathtt{0} & B \\ B^T & \mathtt{0} \end{pmatrix} \tag{7.1}$$

for some matrix B of dimension $k \times \ell$. If $\mathbf{v}$ is an eigenvector for $A(X)$, it can be written as $\mathbf{v} = (\mathbf{v}_1, \mathbf{v}_2)$, where $\mathbf{v}_1 \in \mathbb{R}^k$ and $\mathbf{v}_2 \in \mathbb{R}^\ell$. This partition of the eigenvectors leads to the following lemma.

7.1.1 Lemma. *If θ is an eigenvalue for a bipartite graph X with corresponding eigenvector $(\boldsymbol{v}_1, \boldsymbol{v}_2)$, then $-\theta$ is an eigenvalue with eigenvector $(\boldsymbol{v}_1, -\boldsymbol{v}_2)$.* $\square$

As a consequence, we have the following result.

7.1.2 Lemma. *If X is a bipartite graph and $u \in V(X)$ is a periodic vertex, then no eigenvalue in the support of u is of the form $\frac{a+b\sqrt{\Delta}}{2}$ for non-zero integers a and b with Δ square-free larger than 1.*

Proof. Suppose $\theta = \frac{a+b\sqrt{\Delta}}{2}$ is in the support of u. Then its algebraic conjugate $\overline{\theta} = \frac{a-b\sqrt{\Delta}}{2}$ is also in the support, and by the observation above, the values $-\theta$ and $-\overline{\theta}$ are also eigenvalues in the support of u. If τ is the time at which u is periodic, it follows that $\tau(\theta - \overline{\theta})$ and $\tau(\theta - (-\overline{\theta}))$ are both even multiples of π, a contradiction. $\square$

The following result has been noticed multiple times (see Godsil [35] for more details).

7.1.3 Theorem. *If X is a bipartite graph with a unique perfect matching, then $A(X)$ is invertible and its inverse is an integer matrix. If X is a tree, then $A(X)$ is invertible if and only if X has a (unique) perfect matching.*

As a consequence, we have the following.

7.1.4 Theorem. *Except for K_2, no connected bipartite graph with a unique perfect matching contains periodic vertices.*

Proof. Suppose X is a bipartite graph with a unique perfect matching, and that u is a periodic vertex. Let θ be an eigenvalue in the support of u, and recall from Theorem 2.4.3 that θ is a quadratic integer. By Theorem 7.1.3, $\frac{1}{\theta}$ must be an algebraic integer, and so θ is either $+1$, -1, or of the form $\frac{a+b\sqrt{\Delta}}{2}$ with a and b non-zero. Lemma 7.1.2 excludes the latter case, and hence the only eigenvalues in the support of u are $+1$ and -1. It is easy to see in this case that the connected component containing u is equal to K_2, and so the result follows. □

Note that the corollary below can be used to easily show that no P_n with n even admits perfect state transfer.

7.1.5 Corollary. *Except for K_2, no tree with an invertible adjacency matrix admits perfect state transfer.*

The result above allows us to rule perfect state transfer out of a large class of trees. We can work a bit more in the case where perfect state transfer happens between vertices in different classes of the bipartition.

7.1.6 Lemma. *If X is a bipartite graph admitting perfect state transfer between u and v, and if u and v are in different classes, then their support contains only integer eigenvalues.*

Proof. We prove by contradiction. From Lemma 7.1.2, we need only to consider the case where $b\sqrt{\Delta}$ is in the support of u. From Lemma 7.1.1, if $(\mathbf{v}_1, \mathbf{v}_2)$ is an eigenvector for $b\sqrt{\Delta}$, then $(\mathbf{v}_1, -\mathbf{v}_2)$ is an eigenvector for $-b\sqrt{\Delta}$. Note that $-b\sqrt{\Delta}$ is the algebraic conjugate of $b\sqrt{\Delta}$ in $\mathbb{Q}(\Delta)$, hence $(\mathbf{v}_1, -\mathbf{v}_2)$ is obtained from $(\mathbf{v}_1, \mathbf{v}_2)$ by taking the algebraic conjugate at each entry. As a consequence,

$$(\mathbf{v}_1, \mathbf{v}_2) = (\mathbf{v}_1, \sqrt{\Delta}\mathbf{v}_2'),$$

where $\mathbf{v}_1$ and $\mathbf{v}_2'$ are rational vectors. Thus the absolute value of the entries in the u-th and v-th position are different, and so these vertices cannot be strongly cospectral. □

Now recall Equation 7.1, and observe that it implies that

$$U_A(t) = \begin{pmatrix} \cos(t\sqrt{BB^T}) & \mathtt{i}\sin(t\sqrt{BB^T})B \\ \mathtt{i}\sin(t\sqrt{B^TB})B^T & \cos(t\sqrt{B^TB}) \end{pmatrix}.$$

As a consequence, if perfect state transfer happens in a bipartite graph between vertices in different classes, it must happen with phase $\pm\mathtt{i}$. We use that to prove the following result.

7.1.7 Theorem. *If X is bipartite, perfect state transfer happens between u and v at time τ and u and v belong to different classes, then the eigenvalues in the support of u have the same 2-adic norm. In particular, 0 cannot be in the support of u.*

Proof. We saw that perfect state transfer must happen in this case with phase $\pm\mathtt{i}$. Let θ_0 be the largest eigenvalue of the graph. It is in the support of u, and so it is an integer. If $|\theta_0|_2 = 2^{-\alpha}$, then it follows from Theorem 2.4.4 that τ is an odd multiple of $\frac{\pi}{2^{\alpha+1}}$. Let θ_r be an eigenvector in the support of u, and $\theta_{-r} = -\theta_r$.

Because u and v are in different classes (but are strongly cospectral), $E_r\mathbf{e}_u = \sigma E_r\mathbf{e}_v$ and $E_{-r}\mathbf{e}_u = -\sigma E_{-r}\mathbf{e}_v$ with $\sigma = \pm 1$, and so $\tau(\theta_0 - \sigma\theta_r)$ is an even multiple of π, whereas $\tau(\theta_0 + \sigma\theta_r)$ is an odd multiple of π. All together, we have the following three equations:

$$\begin{aligned} \theta_0 &\equiv 2^\alpha \pmod{2^{\alpha+1}}, \\ \theta_0 - \sigma\theta_r &\equiv 0 \pmod{2^{\alpha+2}}, \\ \theta_0 + \sigma\theta_r &\equiv 2^{\alpha+1} \pmod{2^{\alpha+2}}. \end{aligned}$$

From that it follows that θ_r is also congruent to $2^\alpha \pmod{2^{\alpha+1}}$, and that 0 cannot be in the support of u. □

Conjecture 1. No tree except for P_2 and P_3 admits perfect state transfer.

We checked in `SAGE` that no tree with more than three and less than 11 vertices admits perfect state transfer. We also see the results above as partial steps towards the conjecture. Unfortunately our attempts to move forward have been unfruitful so far, specially on the case where the two vertices belong to the same bipartition class.

7.2 Laplacian matrix

Given a graph X, let $D = D(X)$ be the diagonal matrix whose entries are the degrees of the vertices in X. Recall from Chapter 2 that the *Laplacian matrix* $L = L(X)$ is defined as $L = D - A$.

Suppose each edge $e = uv$ of X is arbitrarily oriented as $\overrightarrow{e} = (u, v)$ or $\overrightarrow{e} = (v, u)$, and let $N = N(X)$ be the oriented incidence matrix of X. That is, for some $u \in V(X)$ and $e \in E(X)$, we have

$$N_{u,e} = \begin{cases} +1, & \text{if } \overrightarrow{e} = (v, u) \text{ for some } v \in V(X), \\ -1, & \text{if } \overrightarrow{e} = (u, v) \text{ for some } v \in V(X), \\ 0, & \text{otherwise.} \end{cases}$$

It follows that $NN^T = L$, and hence L is a positive-semidefinite matrix. For both results below, we refer to Godsil and Royle [42], Chapter 13.

7.2.1 Theorem. *For any graph X with Laplacian matrix L, the following holds.*

(i) The number 0 is an eigenvalue for L. Its multiplicity is equal to the number of connected components of X, and the vector $\boldsymbol{j}$ is always contained in its eigenspace.

(ii) All other eigenvalues of L are positive.

Proof. For (i), it is trivial to notice that $L\mathbf{j} = \mathbf{0}$. If N is defined as above, $L\mathbf{v} = \mathbf{0}$ if and only if $N^T\mathbf{v} = \mathbf{0}$. If X is connected that is true if and only if $\mathbf{v} = \mathbf{j}$. So the multiplicity of 0 as an eigenvalue of L is equal to the number of connected components of X. For (ii), it suffices to note that L is positive-semidefinite. □

7.2.2 Theorem. *Suppose X is a connected graph on n vertices. If $\lambda \neq 0$ is such that $L(X)\boldsymbol{v} = \lambda\boldsymbol{v}$ for some $\boldsymbol{v}$, then $L(\overline{X})\boldsymbol{v} = (n - \lambda)\boldsymbol{v}$. As a consequence, $\lambda \leq n$, and equality holds if and only if $\overline{X}$ is disconnected.*

Proof. The result follows from the fact that $L(\overline{X}) = n\mathtt{I} - \mathtt{J} - L(X)$. □

Perhaps one of the earliest and most important results regarding the Laplacian matrix of a graph is Kirchhoff's Theorem, also called the Matrix Tree Theorem.

7.2.3 Theorem. *Let X be a graph, and u any of its vertices. Let $L[u]$ denote the principal submatrix of $L(X)$ obtained by deleting the row and the column associated to u. Then the number of spanning trees of X is equal to the determinant of $L[u]$.*

As a corollary, we have the following.

7.2.4 Corollary. *Let X be a graph, $0 = \lambda_1 \leq ... \leq \lambda_n$ its Laplacian eigenvalues. Then the number of spanning trees of X is equal to*

$$\frac{1}{n}\prod_{i=2}^{n}\lambda_i.$$

When working with the adjacency matrix, interlacing (Theorem 2.1.13) is very useful to deal with vertex deletion. In the case of the Laplacian matrix, the natural use of interlacing regards edge-deleted subgraphs. The following theorem is folklore.

7.2.5 Theorem. *Let X be a graph, $e \in E(X)$. Suppose the eigenvalues of $L(X)$ are $\lambda_1 \leq ... \leq \lambda_n$, and the eigenvalues of $L(X\backslash e)$ are $\lambda'_1 \leq ... \leq \lambda'_n$. Then*

$$\lambda_i \geq \lambda'_i \geq \lambda_{i-1}.$$

Proof. Let N and M be such that $NN^T = L(X)$, and $MM^T = L(X\backslash e)$. Note that M is obtained from N by removing a column relative to the edge e, and hence M^TM is a principal submatrix of N^TN. Because the positive spectra of AA^T and A^TA are equal for any matrix A, the result now follows from Theorem 2.1.13. □

As a consequence, we have the following.

7.2.6 Corollary. *Let X be a tree on n vertices with Laplacian spectrum $0 = \lambda_1(X) \leq ... \leq \lambda_n(X)$. Then $\lambda_2(X) \leq 1$, and equality holds if and only if X is a star, that is, $X = K_{1,n-1}$.*

Proof. We prove it by induction. If the diameter of X is at most 2, then X is necessarily a star. If the diameter is at least 3, then $|V(X)| \geq 4$, and equal only if $X = P_4$. Note that $\lambda_2(P_4) = 2 - \sqrt{2}$. We suppose by induction that for all trees Y of diameter at least 3 and such that $|V(Y)| < |V(X)|$, we have $\lambda_2(Y) < 1$. Let X be such that $|V(X)| \geq 5$. Then there is an edge e such that one of the components of $X\backslash e$ has diameter at least 3. Let Y be such a component, and so by induction $\lambda_2(Y) < 1$. Note that $\lambda_3(X\backslash e) \leq \lambda_2(Y)$, because $X\backslash e$ has two components, and so the multiplicity of 0 is equal to 2. It follows from Theorem 7.2.5 that $\lambda_3(X\backslash e) \geq \lambda_2(X)$, hence $1 > \lambda_2(X)$.

Finally, the Laplacian spectrum of $K_{1,n-1}$ is $\{0, 1, 1, ..., 1, n-1\}$ (see Example 1 in Merris [59]). $\square$

Definition. The smallest non-zero Laplacian eigenvalue of X is called the *algebraic connectivity* of X, and we will denote it by $a(X)$.

We now present an important result regarding the eigenvectors in the eigenspace of $a(T)$, where T is a tree. It is a combination of a result due to Fiedler [27, Theorem 3.14] and of a result due to Merris [59, Theorem 2].

7.2.7 Theorem. *Let T be a tree and $a(T)$ its smallest non-zero eigenvalue. Then there are two possibilities.*

(i) There is at least one eigenvector $\boldsymbol{v}$ of $a(T)$ such that

$$U = \{u \in V(T) : \boldsymbol{v}_u = 0\} \neq \emptyset.$$

In this case, the subgraph induced by U is connected, and there is only one vertex $w \in V(T)$ in U which is adjacent to a vertex of T not in U. Moreover, if this holds for some eigenvector $\boldsymbol{v}$ of $a(T)$, then it holds for all eigenvectors in the eigenspace of $a(T)$, and w does not depend on the choice of the eigenvector.

(ii) If $\boldsymbol{v}$ is an eigenvector for $a(T)$, and if $\boldsymbol{v}_u \neq 0$ for all $u \in V(T)$, then there is a unique edge uw of T such that $\boldsymbol{v}_u > 0$ and $\boldsymbol{v}_w < 0$. Moreover, if this holds for some eigenvector $\boldsymbol{v}$ of $a(T)$, then it holds for all eigenvectors in the eigenspace of $a(T)$, and the vertices u and w do not depend on the choice of the eigenvector.

Vertices u and w as described in the statement of the theorem are called *characteristic vertices* of the tree. We can classify trees into those satisfying case (i) of Theorem 7.2.7, to be called *type-I trees*; and those satisfying case (ii) of Theorem 7.2.7, to be called *type-II trees*. In particular, type-I trees are those containing one characteristic vertex only, whereas type-II trees contain two characteristic vertices.

We also include a result due to Grone, Merris and Sunder.

7.2.8 Theorem ([44], Theorem 2.1)**.** *Let T be a tree on n vertices, and suppose $\lambda > 1$ is an integer eigenvalue, with a corresponding eigenvector $\boldsymbol{v}$. Then*

(i) λ divides n;

(ii) the multiplicity of λ is 1; and

(iii) no coordinate of $\boldsymbol{v}$ is zero.

To finish this section, we describe the eigenvalues and the eigenvectors of the Laplacian matrix of paths. The following theorem is folklore.

7.2.9 Theorem. *Let $\alpha = \frac{\pi}{n}$. The non-zero eigenvalues of $L(P_n)$ are simple, and for each $k \in \{1, ..., n-1\}$, we have that $(2 - 2\cos(k\alpha))$ is an eigenvalue with corresponding eigenvector*

$$\begin{pmatrix} -\sin(k\alpha) \\ \sin(k\alpha) - \sin(2k\alpha) \\ \sin(2k\alpha) - \sin(3k\alpha) \\ \vdots \\ \sin((n-1)k\alpha) \end{pmatrix}.$$

7.3 Continuous-time quantum walk on the Laplacian matrix

So far we have been considering the quantum walk model where the continuous-time quantum walk is given by $\mathtt{e}^{\mathtt{i}tA}$, where A is the adjacency matrix of the graph. Recall from Equation 2.8 that we can also consider the model in which the continuous-time quantum walk is given by $\mathtt{e}^{\mathtt{i}tL}$, where L is the Laplacian matrix of the graph. Note that if X is k-regular, then both models are equivalent, as $L = k\mathtt{I} - A$, and hence $\mathtt{e}^{\mathtt{i}tL} = \mathtt{e}^{\mathtt{i}tk} \cdot \mathtt{e}^{-\mathtt{i}tA}$.

Because L is a Hermitian matrix, we can use our original definitions of perfect state transfer and periodicity given in Section 2.4. Throughout this section only, whenever we use the terms perfect state transfer, periodicity, strongly cospectral and eigenvalue support relative to a graph X and its vertices, we assume that they refer to the Laplacian matrix of X. Also, in this section only, we will use γ for the phase associated to state transfer, given that the eigenvalues of L will be represented by λ.

Given a graph X with Laplacian matrix L, we will typically represent the spectral decomposition of L by

$$L = \sum_{r=0}^{d} \lambda_r F_r.$$

The eigenvalue support with respect to the Laplacian of a vertex u in X will be denoted by Λ_u.

If u and v are strongly cospectral vertices with respect to the Laplacian, then we define the partiion $\{\Lambda_{uv}^+, \Lambda_{uv}^-\}$ of $\Lambda_u = \Lambda_v$ by the rule

$$\lambda_r \in \Lambda_{uv}^+ \iff F_r \mathbf{e}_u = F_r \mathbf{e}_v \ , \quad \lambda_r \in \Lambda_{uv}^- \iff F_r \mathbf{e}_u = -F_r \mathbf{e}_v.$$

We summarize observations about perfect state transfer with respect to the Laplacian below. Note that this theorem is analogous to Theorem 2.4.4, but stronger in some sense. We emphasize that conditions (ii) and (iii) will follow from simple observations, but both are due to the author.

7.3.1 Theorem. *Let X be a graph, $u, v \in V(X)$. Let $\lambda_0 > ... > \lambda_k$ be the eigenvalues in Λ_u. Then X admits perfect state transfer with respect to the Laplacian from u to v at time τ with phase γ if and only if all of the following conditions hold.*

(i) Vertices u and v are strongly cospectral with respect to the Laplacian.

(ii) Elements in Λ_u are all integers.

(iii) Let $g = \gcd\left(\{\lambda_r\}_{r=0}^{k}\right)$. Then

a) $\lambda_r \in \Lambda_{uv}^+$ if and only if $\dfrac{\lambda_r}{g}$ is even, and

b) $\lambda_r \in \Lambda_{uv}^-$ if and only if $\dfrac{\lambda_r}{g}$ is odd.

Moreover, if these conditions hold, then

a) There is a minimum time $\tau_0 > 0$ such that perfect state transfer with respect to the Laplacian occurs between u and v, and

$$\tau_0 = \frac{\pi}{g}.$$

b) The time τ is an odd multiple of τ_0.

c) The phase γ is equal to 1.

d) Neither u nor v can be involved in perfect state transfer with respect to the Laplacian with a third vertex.

Proof. Suppose $\mathtt{e}^{\mathtt{i}\tau L}\mathbf{e}_u = \gamma\mathbf{e}_v$. Recall that 0 is an eigenvalue of L with corresponding eigenvector $\mathbf{j}$. As a consequence, $0 \in \Lambda_w$ for all $w \in V(X)$. Thus $\lambda_k = 0$. Hence $F_k\mathbf{e}_u = F_k\mathbf{e}_v$, and then $1 = \mathtt{e}^{\mathtt{i}\tau\lambda_k} = \gamma$. Thus $\mathtt{e}^{\mathtt{i}\tau\lambda_r} = \pm 1$, and so $\frac{\lambda_r}{\lambda_s} \in \mathbb{Q}$ for all $r, s \in \{0, ..., k\}$. This only happens if all eigenvalues in Λ_u are integers, or of the form $\lambda_r = t_r\sqrt{\Delta}$ for integers $t_r \in \mathbb{Z}$ and some square-free $\Delta \in \mathbb{Z}$. If $t_r\sqrt{\Delta}$ is an eigenvalue of L, so is its algebraic conjugate $-t_r\sqrt{\Delta}$. However L has no negative eigenvalue, hence all eigenvalues in Λ_u must be integers.

Now $\mathtt{e}^{\mathtt{i}\tau\lambda_r} = 1$ if and only if $\lambda_r \in \Lambda_{uv}^+$, and $\mathtt{e}^{\mathtt{i}\tau\lambda_r} = -1$ if and only if $\lambda_r \in \Lambda_{uv}^-$. A choice of τ satisfying these equations is possible if and only if condition (iii) holds. The other assertions of the statement of the Theorem follow from arguments absolutely analogous to what we did in Chapter 2. □

As a remark, note that the stronger statement below follows from the proof above.

7.3.2 Corollary. *For any graph X with a periodic vertex $u \in V(X)$ with respect to the Laplacian, the eigenvalues in the eigenvalue support of u with respect to the Laplacian must be integers.*

It is clear now why we introduced the results regarding integral Laplacian spectra in the last subsection. We present the consequences.

7.3.3 Corollary. *If a tree T admits perfect state transfer with respect to the Laplacian, then T contains a unique characteristic vertex (that is, T is a type-I tree).*

Proof. No star admits perfect state transfer, so Corollary 7.2.6 implies that $0 < a(T) < 1$. From Theorem 7.3.1, the eigenvalues in the support of vertices involved in perfect state transfer must be integers. So T must be a type-I tree by Theorems 7.2.7 and 7.2.7. $\square$

7.3.4 Corollary. *Except for P_2, no path admits perfect state transfer with respect to the Laplacian.*

Proof. We present two proofs. The direct proof uses Theorem 7.2.9. This result says that all vertices of P_n, except for the middle vertex when n is odd, are in the eigenvalue support of $2 - 2\cos\left(\frac{\pi}{n}\right)$. But that is not an integer unless $n = 2$ or $n = 3$, and it is easy to check that there is no perfect state transfer with respect to the Laplacian in P_3.

The second proof is more sophisticated and uses Corollary 7.3.3. Suppose P_n is a type-I tree. Let $\mathbf{v}$ be an eigenvector for the eigenvalue $a(P_n)$. We know that $\mathbf{j}$ is an eigenvector of $L(P_n)$, hence $\langle \mathbf{v}, \mathbf{j} \rangle = 0$, implying that $\mathbf{v}$ has positive and negative entries. From Theorem 7.2.7 (i), there is a vertex $w \in V(P_n)$ such that $\mathbf{v}_w = 0$, and the entries of $\mathbf{v}$ on every path starting at w are either increasing, decreasing or are constant. Hence the entries to one side of w in P_n are positive, and the entries to the other side are negative. In particular, if P_n is a type-I tree, then only one vertex is not in the support of $a(P_n)$. $\square$

We finish this chapter with a very interesting application of Corollary 7.2.4.

7.3.5 Lemma. *Suppose X is a graph on $n > 2$ vertices admitting perfect state transfer with respect to the Laplacian between u and v. Then Λ_u contains at least one non-zero even eigenvalue, and unless u and v share the same set of neighbours, Λ_u must contain at least three non-zero eigenvalues. Or, more precisely, $|\Lambda_{uv}^+| \geq 2$ and $|\Lambda_{uv}^-| \geq 2$.*

Proof. Let $\Lambda_u = \{\lambda_1, ..., \lambda_k\}$, and $\mathbf{w}^+$ and $\mathbf{w}^-$ be such that

$$\mathbf{w}^+ = \sum_{\lambda_r \in \Lambda_{uv}^+} F_r \mathbf{e}_u \quad \text{and} \quad \mathbf{w}^- = \sum_{\lambda_r \in \Lambda_{uv}^-} F_r \mathbf{e}_u.$$

In particular, $\mathbf{e}_u = \mathbf{w}^+ + \mathbf{w}^-$ and $\mathbf{e}_v = \mathbf{w}^+ - \mathbf{w}^-$, implying that

$$\mathbf{w}^+ = \frac{1}{2}(\mathbf{e}_u + \mathbf{e}_v) \quad \text{and} \quad \mathbf{w}^- = \frac{1}{2}(\mathbf{e}_u - \mathbf{e}_v) \tag{7.2}$$

Consider the situation in which the only even eigenvalue is 0. In view of Theorem 7.3.1, that means that only 0 belongs to Λ^+_{uv}, and hence $\mathbf{w}^+ = \frac{1}{n}\mathbf{j}$. Unless $n = 2$, this contradicts Equation 7.2.

Likewise, if there is only one eigenvalue belonging to Λ^-_{uv}, its corresponding eigenvector is going to be equal to a scalar multiple of $\mathbf{w}^-$, a situation possible only if u and v share the same set of neighbours. □

7.3.6 Theorem. *If X is a graph on an odd number of vertices with an odd number of spanning trees, then perfect state transfer with respect to the Laplacian cannot happen.*

Proof. It follows from Corollary 7.2.4 that X cannot have any even eigenvalue greater than 0. By Lemma 7.3.5, X cannot admit perfect state transfer with respect to the Laplacian. □

7.3.7 Corollary. *No tree on an odd number of vertices admits perfect state transfer with respect to the Laplacian.*

The results in this section suggest that, in some cases, the problem of determining which graphs admit perfect state transfer with respect to the Laplacian might be easier than that with the adjacency matrix.

Conjecture 2. Except for P_2, no tree admits perfect state transfer with respect to the Laplacian.

Chapter 8

Future work

This final chapter is split into short sections, each of them containing some partial (yet new) observations about different aspects related to quantum walks. Our long-term objective is to develop the theory regarding each of these topics.

Section 8.1 is motivated by the question as to which symmetry properties of a graph can be observed from the continuous-time quantum walk matrix. Our best result in this section is obtained by exploring properties of the derivative of $U(t)$, but our work on this topic is still on a early stage. In Section 8.2, we briefly explore another property of the derivative of $U(t)$. Section 8.3 contains yet another equivalent definition of strongly cospectral vertices due to Godsil, and based on that we present some interesting observations. In the last section, we list some problems motivated by the work in this thesis.

8.1 Symmetries of a graph

Recall that a permutation of the vertices of a graph X is an automorphism if and only if $P^T AP = A$, where A is the adjacency matrix of X and P is the associated permutation matrix.

8.1.1 Lemma. *Let X be a graph, and $u, v, w \in V(X)$. If P is a permutation matrix* *representing an automorphism of X such that $P\boldsymbol{e}_u = \boldsymbol{e}_u$ and $P\boldsymbol{e}_v = \boldsymbol{e}_w$, then*

$$U(t)_{u,v} = U(t)_{u,w}$$

for all t.

Proof. Let $U(t) = U_A(t)$. Note that $U_{P^TAP}(t) = U(t)$, but also

$$U_{P^TAP}(t) = P^T U(t) P,$$

and so

$$\begin{aligned} \mathbf{e}_v^T U(t)\mathbf{e}_u &= \mathbf{e}_v^T (P^T U(t) P)\mathbf{e}_u \\ &= (P\mathbf{e}_v)^T U(t)(P\mathbf{e}_u) \\ &= \mathbf{e}_w^T U(t)\mathbf{e}_u. \end{aligned}$$

□

From that, we can derive a simple consequence.

8.1.2 Corollary. *If P is an automorphism that fixes every vertex of the graph and swaps u and v, then if u is involved in perfect state transfer, it must be with v.*

In particular, if a graph Y is obtained from a graph X by appending two vertices v and w of degree 1 adjacent to a vertex $u \in V(X)$, then v and w can only be involved in perfect state transfer with each other. We would like to find a "good" converse of Lemma 8.1.1.

The reason why we are not asking for the proper converse of Lemma 8.1.1 is that it is simply not true. Any asymmetric distance-regular graph will provide one. However, if we require a global hypothesis, we obtain the following.

8.1.3 Theorem. *Let X be a graph, $v, w \in V(X)$. Then $U(t)\boldsymbol{e}_v = U(t)\boldsymbol{e}_w$ for all t if and only if there is a permutation matrix P that swaps v and w and fixes all other vertices of X.*

Proof. One direction is given by Lemma 8.1.1. Now let $A = A(X)$ and suppose the eigenvalues of A are $\theta_0 > ... > \theta_d$. Consider the matrix $U(1)$. Because the eigenvalues of X are algebraic integers, $\mathtt{e}^{\mathtt{i}\theta_i} \neq \mathtt{e}^{\mathtt{i}\theta_j}$ when $i \neq j$. So $U(1)$ has $d+1$ distinct eigenvalues, and hence there is a polynomial $p(x)$ of degree at most d such that $p(U(1)) = A$. Note that for any integer k, $U(1)^k = U(k)$. So the matrices $\{U(k) : k = 0, ..., d+1\}$ form a basis for the algebra spanned by the powers of A. As a consequence of the hypothesis now, $A\mathbf{e}_u = A\mathbf{e}_v$, which is an equivalent statement to what we wanted to prove. Note that the hypothesis could be strengthened to require $U(t)\mathbf{e}_v = U(t)\mathbf{e}_w$ only for a set of $d+1$ distinct algebraic integer values of t, and the same proof would have worked. $\square$

A natural question that arises from the theorem above is whether we can characterize subsets $U \subset V(X)$ such that we need only to assume $U(t)_{u,v} = U(t)_{u,w}$ for $u \in U$ in the hypothesis.

In another direction, we show that under an extra hypothesis we can ignore the complex phase and use only its absolute value.

8.1.4 Theorem. *Let X be a graph, having eigenvalues $\theta_0 > ... > \theta_d$, and let u, v, w be vertices. If, for all times t, we have*

$$|U(t)_{u,v}| = |U(t)_{u,w}|,$$

and, moreover, $(i, j) \neq (k, \ell)$ implies $\theta_i - \theta_j \neq \theta_k - \theta_\ell$, then, for all t,

$$U(t)_{u,v} = U(t)_{u,w}.$$

Proof. The first hypothesis is equivalent to

$$|\mathbf{e}_v^T U(t)\mathbf{e}_u|^2 = |\mathbf{e}_w^T U(t)\mathbf{e}_u|^2.$$

We have

$$\begin{aligned}
|\mathbf{e}_v^T U(t)\mathbf{e}_u|^2 &= \left(\sum_{r=0}^{d} \mathtt{e}^{\mathtt{i}\theta_r t}(\mathbf{e}_v^T E_r \mathbf{e}_u)\right)\left(\sum_{r=0}^{d} \mathtt{e}^{-\mathtt{i}\theta_r t}(\mathbf{e}_v^T E_r \mathbf{e}_u)\right) \\
&= \sum_{r=0}^{d} (\mathbf{e}_v^T E_r \mathbf{e}_u)^2 + 2\sum_{r<s} (\mathbf{e}_v^T E_r \mathbf{e}_u)(\mathbf{e}_v^T E_s \mathbf{e}_u)\cos(t(\theta_r - \theta_s)).
\end{aligned}$$

Note that this is an analytical function on $t \in \mathbb{R}^+$. If two functions are identical, then the same holds for their derivatives. It follows that

$$\frac{\mathrm{d}^n}{\mathrm{d}t^n}\ |\mathbf{e}_v^T U(t) \mathbf{e}_u|^2 = \frac{\mathrm{d}^n}{\mathrm{d}t^n}\ |\mathbf{e}_w^T U(t) \mathbf{e}_u|^2. \tag{8.1}$$

If we denote

$$F(t; r, s) = \sin(t(\theta_r - \theta_s))\big[(\mathbf{e}_v^T E_r \mathbf{e}_u)(\mathbf{e}_v^T E_s \mathbf{e}_u) - (\mathbf{e}_w^T E_r \mathbf{e}_u)(\mathbf{e}_w^T E_s \mathbf{e}_u)\big],$$

then Equation 8.1 implies that

$$\sum_{r<s} (\theta_r - \theta_s)^n F(t; r, s) = 0$$

for all positive odd integers n.

Using now the second hypothesis, and taking sufficiently large n, we can conclude that for all r, s and for all t,

$$F(t; r, s) = 0$$

This is equivalent to

$$(\mathbf{e}_v^T E_r \mathbf{e}_u)(\mathbf{e}_v^T E_s \mathbf{e}_u) = (\mathbf{e}_w^T E_r \mathbf{e}_u)(\mathbf{e}_w^T E_s \mathbf{e}_u)$$

for all r and s.

Comparing such equalities for three indices r, s and q, and given that the projector E_0 is a positive matrix, it must be the case that

$$\mathbf{e}_v^T E_r \mathbf{e}_u = \mathbf{e}_w^T E_r \mathbf{e}_u$$

for all r, and so

$$\mathbf{e}_v^T U(t) \mathbf{e}_u = \mathbf{e}_w^T U(t) \mathbf{e}_u.$$

□

Another way of overcoming the fact that the converse of Lemma 8.1.1 is not true is to consider a relaxation of the definition of automorphism.

Definition. Given a graph X, $A = A(X)$, an orthogonal matrix Q that commutes with A is called a *symmetry* of X.

Recall from the end of Chapter 2 that we already considered such matrices. In view of the theory we build up then, we have the following result.

8.1.5 Corollary. *Let X be a graph with vertices u, v and w. Then v and w are cospectral and $U(t)_{u,v} = U(t)_{u,w}$ for all t if and only if there is a symmetry of X that swaps v and w but fixes u.*

Proof. From Theorem 2.5.1, v and w are cospectral if and only if there is a symmetry Q such that $Q^2 = \mathtt{I}$ and $Q\mathbf{e}_v = \mathbf{e}_w$. Note that if $U(t)_{u,v} = U(t)_{u,w}$, then it follows from the proof of Theorem 8.1.3 that $(E_r)_{u,v} = (E_r)_{u,w}$ for all r. Hence $\langle \{A^k \mathbf{e}_u\}_{k \geq 0} \rangle$ is orthogonal to $\langle \{A^k(\mathbf{e}_v - \mathbf{e}_w)\}_{k \geq 0} \rangle$. From the definition of Q, this implies that $Q\mathbf{e}_u = \mathbf{e}_u$.

On the other hand, we have that $Q^T U(t) Q = U(t)$, and if Q fixes u, we have, for all t,

$$\mathbf{e}_u^T U(t) \mathbf{e}_w = (\mathbf{e}_u^T Q^T) U(t) (Q\mathbf{e}_v) = \mathbf{e}_u^T (Q^T U(t) Q) \mathbf{e}_v = \mathbf{e}_u^T U(t) \mathbf{e}_v.$$

□

8.2 The derivative of $U(t)$

Recall from Chapter 3 that the Schur product of matrices M and N is entry-wise defined as $(M \circ N)_{ab} = M_{ab} \cdot N_{ab}$. In terms of the Schur product, we can say that a graph X admits perfect state transfer from u to v if and only if

$$(U(t) \circ U(-t))_{uv} = 1.$$

Note that a necessary condition for this to happen is that the u-th column of the (entry-wise) derivative of $U(t) \circ U(-t)$ is 0. In that direction, we have the following result.

8.2.1 Theorem. *Let X be a graph, $u \in V(X)$. Then $\dfrac{\mathrm{d}}{\mathrm{d}t}(U(t) \circ U(-t))\ \boldsymbol{e}_u = \boldsymbol{0}$ if and only if the restriction of $U(t)\boldsymbol{e}_u$ to its non-zero entries is a vector that lies in the kernel of the adjacency matrix of the subgraph induced by such entries.*

Proof. First recall that $U(t)$ is a polynomial in t with matrix coefficients, and hence the derivative of $U(t)$ with respect to t is the matrix whose entries are the derivatives of the polynomials in t that correspond to the entries of $U(t)$. It is not difficult to see that, after some re-arrangement, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}U(t) = \mathtt{i}AU(t).$$

Now, by the product rule,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(U(t) \circ U(-t)) &= (\mathtt{i}AU(t)) \circ U(-t) + U(t) \circ (-\mathtt{i}AU(-t)) \\ &= (\mathtt{i}AU(t)) \circ U(-t) + \overline{(\mathtt{i}AU(t)) \circ U(-t)}.\end{aligned}$$

But recall that this is a real matrix, hence the u-th column is 0 if and only if

$$\big[(\mathtt{i}AU(t)) \circ U(-t)\big]\mathbf{e}_u = \mathbf{0}.$$

That is true if and only if $(\mathtt{i}AU(t)\mathbf{e}_u) \circ (U(-t)\mathbf{e}_u) = \mathbf{0}$, which in turn is equivalent to $AU(t)\mathbf{e}_u$ and $U(t)\mathbf{e}_u$ having disjoint supports. Let Y be the subgraph induced by the vertices whose corresponding entry in $U(t)\mathbf{e}_u$ is non-zero. Then $AU(t)\mathbf{e}_u$ and $U(t)\mathbf{e}_u$ have disjoint supports if and only if the restriction of $U(t)\mathbf{e}_u$ to Y is an eigenvector of Y with eigenvalue 0. □

From that, we derive two more intelligible corollaries.

8.2.2 Corollary. *Let X be a graph, $u \in V(X)$. If the support of $U(t)\boldsymbol{e}_u$ is an independent set of X, then $\frac{\mathrm{d}}{\mathrm{d}t}(U(t) \circ U(-t))\ \boldsymbol{e}_u = \boldsymbol{0}$.*

8.2.3 Corollary. *Let X be a graph, $u \in V(X)$. If $\frac{\mathrm{d}}{\mathrm{d}t}(U(t) \circ U(-t))\ \boldsymbol{e}_u = \boldsymbol{0}$, then the subgraph of X spanned by the support of $U(t)\boldsymbol{e}_u$ must have the eigenvalue 0.*

8.3 Other properties of strongly cospectral vertices

The main question inspiring this section is to determine what is the maximum size of a subset of the vertices of a graph that are pairwise strongly cospectral.

We would have liked the answer of this question to be 2, but (unpublished) computations carried by Fidel Barrera-Cruz found some examples of regular graphs on few vertices containing a set of 3 vertices that are pairwise strongly cospectral. We then turn our attention to answering the problem by finding an upper bound. The following lemma generalizes a (unpublished) result due to Godsil.

8.3.1 Lemma. *Let X be a graph on n vertices with eigenvalues $\{\theta_r\}_{r=0}^{d}$. Let $\{u_1, ..., u_k\} \subset V(X)$, and $\mathbf{e}_i$ the characteristic vector of u_i. If these vertices are parallel, then for all eigenvalues θ_r of X with multiplicity m_r, the multiplicity of θ_r in $X \backslash \{u_1, ..., u_k\}$ is at least $m_r - 1$.*

Proof. Let S_r be the eigenspace of $A(X)$ associated to θ_r. These vertices are parallel if and only if, for all $r \in \{0, ..., d\}$, the subspace

$$T_r = \text{span}\,\{E_r\mathbf{e}_i\}_{i=1}^{k}$$

has dimension at most 1. This is equivalent to saying that the quotient subspace S_r/T_r has dimension at least $m_r - 1$. But this subspace is isomorphic to a subspace of the eigenspace of θ_r in the matrix $A(X\backslash\{u_1, ..., u_k\})$. □

This lemma directly implies the best known bound for the maximum size of a subset of the vertices of a graph that are parallel with the same eigenvalue support, in particular it is the best answer we have for the question motivating this section.

8.3.2 Theorem. *Given a vertex u in X, the maximum number of vertices that are parallel to u and whose eigenvalue support is contained in the eigenvalue support of u is at most equal to the size of the eigenvalue support of u.*

We now introduce a different approach, partly based on the following results due to Godsil [40]. We will use the notation $M^{\circ 2} = M \circ M$.

8.3.3 Lemma. *Given a graph X with eigenvalues $\{\theta_r\}_{r=0}^{d}$, and $u, v \in V(X)$, we have that u and v are strongly cospectral if and only if, for all r, ${E_r}^{\circ 2}\ \mathbf{e}_u = {E_r}^{\circ 2}\ \mathbf{e}_v$.*

Proof. It follows trivially from observing that ${E_r}^{\circ 2}\ \mathbf{e}_u = E_r\mathbf{e}_u \circ E_r\mathbf{e}_u$. □

8.3.4 Theorem ([40], Theorem 9.3)**.** *If $\lambda_r > 0$ for all r, then vertices u and v are strongly cospectral if and only if*

$$\sum_{r=0}^{d} \lambda_r {E_r}^{\circ 2} \, (\boldsymbol{e}_u - \boldsymbol{e}_v) = \boldsymbol{0}. \tag{8.2}$$

Proof. If u and v are strongly cospectral, Lemma 8.3.3 trivially implies Equation 8.2.

For the converse, note that the matrix E_r is positive-semidefinite, hence by Schur's Theorem ([64], Theorem VII), we have that ${E_r}^{\circ 2}$ is positive-semidefinite. As a consequence, $(\mathbf{e}_u - \mathbf{e}_v)^T {E_r}^{\circ 2} \, (\mathbf{e}_u - \mathbf{e}_v) \geq 0$. From Equation 8.2,

$$(\mathbf{e}_u - \mathbf{e}_v)^T \sum_{r=0}^{d} \lambda_r {E_r}^{\circ 2} \, (\mathbf{e}_u - \mathbf{e}_v) = 0,$$

thus $(\mathbf{e}_u - \mathbf{e}_v)^T {E_r}^{\circ 2} \, (\mathbf{e}_u - \mathbf{e}_v) = 0$ for all r. Hence

$$[(E_r)_{u,u}]^2 + [(E_r)_{v,v}]^2 - 2[(E_r)_{u,v}]^2 = 0. \tag{8.3}$$

Given that ${E_r}^{\circ 2}$ is a positive-semidefinite matrix, and hence a Gram matrix, the Cauchy-Schwarz inequality implies that

$$[(E_r)_{u,u}]^2 [(E_r)_{v,v}]^2 - [(E_r)_{u,v}]^4 \geq 0. \tag{8.4}$$

Equations 8.3 and 8.4 imply that

$$[(E_r)_{u,u}]^2 = [(E_r)_{v,v}]^2 = [(E_r)_{u,v}]^2.$$

Recall that E_r is an idempotent, hence $(E_r)_{u,v} = \langle E_r \mathbf{e}_u, E_r \mathbf{e}_v \rangle$. Therefore, by Cauchy-Schwarz again, we have, for all r,

$$E_r \mathbf{e}_u = \pm E_r \mathbf{e}_v.$$

$\square$

Recall from Chapter 6 that for each graph X with $d+1$ distinct eigenvalues, we can define a sequence of orthogonal polynomials $p_0(x), ..., p_d(x)$ with respect to the trace inner product. Theorem 6.1.2 implies that

$$\sum_{r=0}^{d} \frac{1}{m_r}\ E_r \otimes E_r = \sum_{r=0}^{d} \frac{1}{\operatorname{tr} p_r(A)^2}\ p_r(A) \otimes p_r(A). \tag{8.5}$$

Therefore:

8.3.5 Theorem. *Given a graph X, vertices u and v, and orthogonal polynomials $p_0(x), ..., p_d(x)$, it follows that u and v are strongly cospectral if and only if*

$$\sum_{r=0}^{d} \frac{1}{\operatorname{tr} p_r(A)^2}\ p_r(A) \circ p_r(A)\ (\boldsymbol{e}_u - \boldsymbol{e}_v) = \boldsymbol{0}.$$

Proof. Follows from Theorem 8.3.4, Equation 8.5, and the fact that for any matrix M, $M \circ M$ is a submatrix of $M \otimes M$. □

We believe that this theorem might provide a good way of testing whether two vertices are strongly cospectral, or in bounding how many vertices can be pairwise strongly cospectral. We believe this is even more strongly in the context of association schemes or coherent configurations, where the matrices $p_r(A)$ have a combinatorial meaning.

8.4 Compilation of problems

Problem 1. Characterize which trees admit perfect state transfer with respect to the adjacency matrix.

Problem 2. Characterize which trees admit perfect state transfer with respect to the Laplacian matrix.

In Chapter 7, we showed some advance in both problems above. All of our results indicated classes of trees in which perfect state transfer cannot happen, and so we conjectured that the answer to the first problem might be P_2 and P_3 only, whereas for the second problem that would be P_2 only.

Problem 3. Characterize the translation graphs that admit perfect state transfer.

Our work on association schemes in Chapter 3, on products in Chapter 4 and on two classes of translation graphs in Chapter 5 can be seen as a partial progress towards solving the problem above. The problems below are also inspired by our work in Chapter 5.

Problem 4. Find an efficient way of checking whether a cubelike graph $(\mathbb{Z}_2^d, \mathcal{C})$ with $\sum_{g \in \mathcal{C}} g = 0$ admits perfect state transfer.

Problem 5. Find more examples of cubelike graphs admitting perfect state transfer at arbitrarily small times.

Problem 6. Find a more elementary proof of Theorem 5.2.2.

In the other sections of this chapter, we motivated the problems below.

Problem 7. Find a "good" converse for Lemma 8.1.1.

Problem 8. To what extent can the seemingly unnatural hypothesis on the differences of the eigenvalues in Theorem 8.1.4 be weakened?

Problem 9. What is the maximum size of a subset of the vertices of a graph that are pairwise strongly cospectral?

Finally, we state a problem somewhat related to the problem of determining which trees admit perfect state transfer.

Problem 10. If X is a graph of diameter d, what is the minimum number of edges (as a function of d) needed to achieve perfect state transfer between vertices at distance d ?

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