Algebraic aspects of
Multi-Particle Quantum Walks

by

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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.

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Abstract

A continuous time quantum walk consists of a particle moving among the vertices of a graph G. Its movement is governed by the structure of the graph. More formally, the adjacency matrix A is the Hamiltonian that determines the movement of our particle. Quantum walks have found a number of algorithmic applications, including unstructured search, element distinctness and Boolean formula evaluation. We will examine the properties of periodicity and state transfer. In particular, we will prove a result of the author along with Godsil, Kirkland and Severini [28], which states that pretty good state transfer occurs in a path of length n if and only if the $n+1$ is a power of two, a prime, or twice a prime. We will then examine the property of strong cospectrality, a necessary condition for pretty good state transfer from u to v.

We will then consider quantum walks involving more than one particle. In addition to moving around the graph, these particles interact when they encounter one another. Varying the nature of the interaction term gives rise to a range of different behaviours. In particular, the particles can take on the characteristics of Fermions or Bosons. We will introduce a graph invariant proposed by Gamble, Friesen, Zhou, Joynt and Coppersmith [22]. This invariant takes the entries of the k-particle transition matrix as a list. A second invariant, due to Emms, Hancock, Severini and Wilson [17], is based on the discrete time quantum walk on a graph. One of the objectives of the sections that follow will be to characterize the strength of these two graph invariants.

Cellular algebras are complex-valued matrix algebras that are closed under Schur multiplication and transposition. They were first studied by Weisfeiler and Lehman [40], as well as Higman [30]. With any graph G, we can associate a cellular algebra $W = W(G)$. We define the k-extension $\widehat{W}^{(k)}$ of W for any positive integer k. We show that, if two graphs yield isomorphic k-extensions, then the k-particle invariant of Gamble et al. cannot distinguish the graphs. Similarly, if the 2-extensions of a pair of graphs are isomorphic, the invariant of Emms et al. cannot distinguish them. Finally, we give constructions for pairs of non-isomorphic graphs with isomorphic k-extensions for any positive integer k. Both of these results, along with the constructions, are the work of the author.

Let $\mathcal{A}$ be an association scheme of $n \times n$ matrices. Then, any element of $\mathcal{A}$ can act on the space of $n \times n$ matrices by left multiplication, right

multiplication, and Schur multiplication. The set containing these three linear mappings for all elements of $\mathcal{A}$ generates an algebra. This is an example of a Jaeger algebra. Although these algebras were initially developed by François Jaeger in the context of spin models and knot invariants, they prove to be useful in describing multi-particle walks as well. We will focus on triply-regular association schemes, proving several new results regarding the representation of their Jaeger algebras. As an example, we present the simple modules of a Jaeger algebra for the 4-cube.

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For Martine. And the Bean.

Contents

Chapter 1

Introduction

A random walk in continuous time on a graph $G = (V, E)$ is can be described by a matrix L whose entries are given by

$$L_{uv} = \begin{cases} 1 & uv \in E \\ -\deg(u) & u = v \\ 0 & \text{otherwise.} \end{cases}$$

The state of the walk at time t is denoted by $\mathbf{x}(t)$, a probability distribution on the vertices of G. The evolution of the walk is given by the walk is given by the equation

$$\frac{d}{dt}\mathbf{x}(t) = L\mathbf{x}(t).$$

This gives us

$$\mathbf{x}(t) = e^{Lt}\mathbf{x}(0).$$

Random walks—in both discrete and continuous time—have found extensive applications in the simulation of biological and physical systems, as well as algorithms such Monte Carlo methods and the Metropolis algorithm.

To define a continuous-time quantum walk, we replace the Markovian dynamics of the random walk with quantum dynamics. The walk is described by a symmetric *Hamiltonian*. For our purposes, we will use the adjacency matrix A of the graph G. The state of the walk is given by a complex vector $\mathbf{x}$ of unit length. The evolution of the walk is given by

$$i\frac{d}{dt}\mathbf{x}(t) = A\mathbf{x}(t).$$

Solving, we get

$$\mathbf{x}(t) = e^{-iAt}\mathbf{x}(t).$$

Since A is symmetric, e^{-iAt} is a unitary operator, which we denote by $U(t)$. The continuous-time quantum walk was first defined by Farhi and Guttmann in [21]. The discrete-time quantum walk has also received a great deal of attention (see [38],[34]). Quantum walks have found a large range of algorithmic applications. In 2002, Childs, Cleve, Deotto, Farhi, Guttmann and Spielman [12] showed that certain graphs can be traversed exponentially faster by a quantum walk than its classical counterpart. Other well-known applications of quantum walks include unstructured search ([34], [36]), spatial search [11] and element distinctness [3]. In Chapter 3, we give a detailed definition and description of continuous-time quantum walks.

It is possible to relate many physical properties of the quantum walk to the structure of the underlying graph. Let e_v denote the v^{th} elementary vector, consisting of a 1 in the v^{th} place and zeros everywhere else. A graph exhibits *perfect state transfer* from u to v at time t if

$$U(t)e_u = \beta e_v$$

for some complex phase factor β. We say that a graph has *pretty good state transfer* from u to v if there is a unit complex number β such that, for any $\delta > 0$, there is some time t_δ such that

$$|e_v U(t_\delta) e_u - \beta| < \delta.$$

That is, the quantum walk comes arbitrarily close to achieving perfect state transfer. In [26], Godsil provides many of the definitions and fundamental results that we will draw upon. State transfer has substantial implications for the transfer of information between networked quantum mechanical sites, and are therefore applicable to the design of hardware for quantum communication and computation. For example, Bose [8] considered the transfer of a state between the endpoints of a path. In joint work of the author, Godsil, Kirkland and Severini [28], it is shown that pretty good state transfer occurs on the path of length n if and only if $n + 1$ is a prime, twice a prime, or a power of two. A consequence of this result is the surprising connection between detecting pretty good state transfer and primality testing.

A natural extension of the continuous-time quantum walk allows for multiple walkers or particles. These particles interact with each other while moving about the graph. The Hamitonian for a multi-particle walk consists of a movement term M and an interaction term N:

$$H = M + N.$$

Altering the interaction term can produce dramatic variations in the dynamics of the walk. The most common choice for N simply applies an energy penalty b for each pair of particles that are located at the same vertex. It is also interesting to consider multi-particle walks restricted to the symmetric or anti-symmetric subspaces. The particles described by these restriction are, respectively, Bosons and Fermions. The dynamics of these walks can reveal a great deal about the features of the underlying graph, suggesting that they might offer an approach to the graph isomorphism problem

An isomorphism from a graph G to H is a bijection

$$\phi : V(G) \to V(H)$$

such that

$$(u, v) \in E(G) \Leftrightarrow \big(\phi(u), \phi(v)\big) \in E(H).$$

The *graph isomorphism problem* asks us to decide whether or not a pair of graphs is isomorphic. The graph isomorphism problem has attracted a great deal of attention, because of both its wide-ranging applications and its complexity. While there is no known polynomial time algorithm for graph isomorphism, it is also not known to be NP-complete. The best known algorithm, due to Luks and Babai [5], solves the graph isomorphism problem on a graph with n vertices in $2^{O(\sqrt{n \log n})}$ time.

A common approach to the graph isomorphism problem is to calculate a *graph invariant*. An invariant is a function of a graph f such that, if G and H are isomorphic, then $f(G) = f(H)$. If $f(G) = f(H)$ only when G and H are isomorphic, we say that f is *complete*. Clearly, computing a complete graph invariant solves the graph isomorphism problem.

Gamble, Friesen, Zhou, Joynt, and Coppersmith propose a graph invariant that is based on a 2-Boson quantum walk. They show computationally that using two Bosons yields strictly greater distinguishing power than the single-particle walk [22]. Emms, Hancock, Severini and Wilson describe an invariant based on the discrete-time quantum walk [17], and conjecture that it is strong enough to distinguish all strongly regular graphs. It should be noted that, while both of these invariants are based on quantum walks, they are classical algorithms. That is, they involve either simulating a quantum walk or calculating relevant properties classically. The exact strength of these two invariants is an open question.

Our initial motivation was to characterize the strength of these two invariants; this thesis contains several results to this end. However, proving them has led to a far broader research agenda. Central to this agenda is the application of algebraic tools—such as association schemes and cellular algebras—to the description and analysis of quantum walks. We will now outline the organization of this thesis, highlighting the major questions we will address, as well as some significant results.

1.1 Organization of the Thesis

In this thesis, we introduce a number of algebraic tools and apply them to the study of quantum walks. We examine some fundamental properties of single particle quantum walks and their relation to the underlying graph. We then consider multi-particle walks; in particular, we identify limitations on the effectiveness of the invariants of Gamble et al., as well as that of Emms et al. Finally, we return to the two particle case. We show that the two particle walk is related to matrix algebras called *Jaeger algebras*, and develop the representation theory of these algebras.

In Chapter 2, we will introduce association schemes and semisimple algebras. A symmetric association scheme $\mathcal{A}$ is a set of symmetric 01-matrices such that contains the identity, sums to the all-ones matrix, and whose span is closed under matrix multiplication. We introduce some of the useful properties of association schemes and show that a distance regular graph G gives rise to an association scheme with $A_1 = A(G)$.

Let $\mathcal{B}$ be an algebra acting on a vector space V. A $\mathcal{B}$-module is a subspace of V that is invariant under the action of $\mathcal{B}$. A module is simple if it contains no $\mathcal{B}$-module other than 0 and itself. We say that a module is *semisimple* if V can always be decomposed into a sum of simple $\mathcal{B}$-modules. In this case, we can write the action of $\mathcal{B}$ on V as the direct sum of its action on each of the modules. This can often greatly simplify our analysis of the action of $\mathcal{B}$. In Chapter 2, we define semisimple algebras in detail and prove some fundamental results about their structure. These results will prove useful in our discussion of Jaeger algebras in Chapter 5.

In Chapter 3, we introduce continuous-time quantum walks and the notions of perfect state transfer and pretty good state transfer. We establish a new necessary and sufficient condition for perfect state transfer in a graph whose eigenvalues are rational multiples of some algebraic integer. We also review a result of the author, along with Kirkland, Godsil, and Severini [28], which says that pretty good state transfer occurs between the endpoints of the path on n vertices if and only if n is a prime, twice a prime, or a power of two. This result highlights a surprising connection between number theory and the physics of quantum walks.

In order for a pair of vertices to exhibit perfect state transfer or pretty good state transfer, they must be *strongly cospecral*, a property that we will define and examine in detail in Section 3.1.3. We give necessary and sufficient conditions for two vertices to be strongly cospectral, and establish a bound on the number of pairwise strongly cospectral vertices in a graph. Next, we show that, if u and v are strongly cospectral in G, then there is a matrix X with eigenvalues ± 1 that is a polynomial in A and swaps u and v. We use this result to prove strong conditions on strongly cospectral vertices in distance regular graphs. We also provide a construction that, given a graph G with cospectral vertices u and v, produces a graph H with strongly cospectral vertices u' and v'.

In Section 3.2, we introduce multi-particle quantum walks. We develop a description of multi-particle walks that is as general as possible, while still respecting the structure of the underlying graph. Lastly, we describe the k-Boson invariant of Gamble, Friesen, Zhou, Joynt and Coppersmith [22] along with the invariant of Emms, Severini and Wilson [17], which is based on a discrete time quantum walk.

In Chapter 4, we define cellular algebras, which generalize association schemes. We show that each graph can be associated with a cellular algebra, called its cellular closure. We define the k-extension of a cellular algebra and mappings between these extensions, called k-isomorphisms. Two graphs are said to be k-equivalent if they are contained in cellular algebras that are related by a k-isomorphism. In Theorem 4.5.4, we show that, if two graphs are k-equivalent, then the k-particle quantum walks on these graphs share many characteristics. In particular, k-equivalent pairs of graphs are not distinguished by the k-Boson invariant of Gamble et al. We prove analogous results for discrete time walks as well, demonstrating that pairs of 2-equivalent graphs are not distinguished by the invariant of Emms et al. Finally, we give a construction for pairs of non-isomorphic k-equivalent graphs for all k. Emms et al. conjecture that their invariant distinguishes all pairs of non-isomorphic strongly regular graphs. While the construction presented here is not strongly regular, it has diameter two and four eigenvalues; in this sense it is "close."

In Chapter 5, we analyze two particle quantum walks using Jaeger algebras. These algebras were first recognized by François Jaeger in the context of spin models. The relevant excerpt of his unpublished notes is reproduced in Section 5.5.4. Our objective in this Chapter 5 is to identify the simple modules of the Jaeger algebra of a graph G. In doing so, we can decompose a high-dimensional walk into the sum of walks on the simple modules, which may have much smaller dimension. This decomposition can facilitate, for example, computing the evolution of the walk in parallel. Theorems 5.5.8, 5.5.9 and 5.5.17, along with Lemmas 5.5.11-5.5.15 provide some of the required tools for identifying these modules. We apply these results to the representation of the 4-cube, and provide a complete list of the simple modules of its Jaeger algebra $\mathcal{J}_4$.

Chapter 2

Algebraic Preliminaries

In this chapter, we will introduce *association schemes* and *semisimple algebras*. Each will play an important role in subsequent chapters. The definitions and results presented here are well-known; only the presentation is new.

2.1 Association Schemes

The treatment of association schemes in this section draws on Godsil's notes ([23]), as well as the work of Bannai and Ito ([7]); additional details on this topic can be found there. An *association scheme* is a set of 01-matrices $\mathcal{A} = \{A_0, ..., A_\ell\}$ indexed by a vertex set $\mathbf{V} = \{v_1, ..., v_n\}$ such that

(i) $A_0 = I$.

(ii) $\sum_i A_i = J$.

(iii) $A_i^T \in \mathcal{A}$ for all i.

(iv) There are constants p_{ij}^k such that

$$A_i A_j = A_j A_i = \sum_k p_{ij}^k A_k.$$

Each $n \times n$ matrix A_i defines a binary relation R_i on V and we say that $uv \in R_i$ whenever $(A_i)_{uv} = 1$. We refer to the matrices $A_1, ..., A_\ell$ (or their corresponding $R_1, ..., R_\ell$) as the *basis relations* of the association scheme $\mathcal{A}$.

When $A_i = A_i^T$ for all i, we say that $\mathcal{A}$ is a *symmetric association scheme*. The values p_{ij}^k are called the *intersection numbers* of the association scheme.

A *Bose-Mesner algebra* is the complex span of an association scheme, $\mathbb{C}[\mathcal{A}]$. We define *Schur multiplication* as follows:

$$(M \circ N)_{ij} = M_{ij} N_{ij}.$$

In addition to being closed under matrix multiplication and transposition, a Bose-Mesner algebra is closed under Schur multiplication.

We say that an operator M is *normal* if

$$MM^* = M^*M,$$

where M^* denotes the adjoint of M—in this case, the complex transpose. The following theorems are well-known:

2.1.1 Theorem. *If N is a normal operator, then it can be written as a linear combination of orthogonal idempotents $E_0, ..., E_k$:*

$$M = \sum_j a_j E_j. \qquad \square$$

2.1.2 Theorem. *Two normal operators M and N commute if and only if there is an orthogonal set of idempotents $E_0, ..., E_k$ such that*

$$M = \sum_j a_j E_j, \qquad N = \sum_j b_j E_j. \qquad \square$$

Requirements (iii) and (iv) tell us that $\mathbb{C}[\mathcal{A}]$ consists of commuting normal operators. Therefore, there exists a minimal set of orthogonal idempotents $\mathcal{E} = \{E_0, ..., E_k\}$ that span $\mathbb{C}[\mathcal{A}]$. In particular, there are values $p_i(j)$ such that

$$A_i = \sum_j p_i(j) E_j.$$

The values $p_i(j)$ are the *eigenvalues* of $\mathcal{A}$.

2.1.3 Lemma. *The set $\mathcal{E}$ is a basis for $\mathbb{C}[\mathcal{A}]$.*

Proof. We know that $\mathcal{E}$ spans $\mathbb{C}[\mathcal{A}]$, so we need only show that every E_i is contained in $\mathbb{C}[\mathcal{A}]$. First, we note that for every distinct pair E_j, E_k, there is some A_i in $\mathcal{A}$ such that $p_i(j) \neq p_i(k)$. If not, then the set $\mathcal{E}$ would not be minimal. As a result, there is some $M \in \mathbb{C}[\mathcal{A}]$ such that

$$M = \sum_i a_i E_i$$

and the a_i are all distinct. It is then easy to verify that

$$\prod_{i \neq j}(M - a_i I) = \prod_{i \neq j}(a_j - a_i)E_j.$$

Therefore, $E_j \in \mathcal{A}$ for all j. The set $\mathcal{E}$ is a basis for $\mathcal{A}$ and $k = \ell$. $\square$

Lemma 2.1.3 has two immediate consequences. Firstly, there are scalars q_{ij}^k such that

$$E_i \circ E_j = \frac{1}{n} \sum_j q_{ij}^k E_k.$$

The values q_{ij}^k are called the *Krein parameters* of the scheme $\mathcal{A}$. Secondly, there are scalars $q_i(j)$ such that

$$E_i = \frac{1}{n} \sum_j q_i(j) A_j.$$

The values $q_i(j)$ are the *dual eigenvalues* of $\mathcal{A}$. If we define matrices P and Q such that

$$P_{i,j} = p_j(i), \qquad Q_{i,j} = q_j(i),$$

then we have

$$PQ = nI.$$

We say that an association scheme is P-polynomial with respect to the ordering $A_0, ..., A_\ell$ of basis relations if, for each i, there is a polynomial ϕ_i of degree i such that

$$A_i = \phi_i(A_1).$$

We can restate this in terms of the eigenvalues of $\mathcal{A}$:

$$p_i(j) = \phi_i(p_1(j)).$$

A *Schur polynomial* is one in which Schur multiplication takes the place of matrix multiplication. An association scheme is Q-polynomial relative to an ordering $E_0, ..., E_\ell$ if, for each i, there is a Schur polynomial ψ_i of degree i such that

$$E_i = \psi_i(E_1).$$

This can be expressed in terms of dual eigenvalues as follows:

$$q_i(j) = \psi_i(q_1(j)).$$

We will now describe a well-known source of P-polynomial association schemes—distance-regular graphs.

2.1.1 Example: distance regular graphs

A graph G of diameter d is *distance regular* if there are constants

$$a_i, b_i, c_i \qquad i = 0, ..., d$$

such that, for any pair of vertices u, v at distance i, there are exactly

- a_i vertices at distance 1 from u and i from v,
- b_i vertices at distance 1 from u and $i+1$ from v, and
- c_i vertices at distance 1 from u and $i-1$ from v.

Note that such a graph is regular with degree b_0.

2.1.4 Lemma. *Let $G = (V, E)$ be a distance regular graph and A_i be a 01-matrix indexed by V such that*

$$(A_i)_{uv} = \begin{cases} 1 & d(u,v) = i \\ 0 & \textit{otherwise.} \end{cases}$$

Then $\mathcal{A} = \{A_0, ..., A_d\}$ is a P-polynomial association scheme.

Proof. Clearly, A_0 and A_1 can be expressed as polynomials in A_1. Assume that $A_i = \phi_i(A_i)$ for all $i \leq j$. Then,

$$A_1 A_j = b_{j-1} A_{j-1} + a_j A_j + c_{j+1} A_{j+1}$$

and therefore

$$A_{j+1} = \frac{1}{c_{j+1}} \left(A_1 \phi_j(A_1) - b_{j-1} \phi_{j-1}(A_1) - a_j \phi_j(A_1) \right).$$

So A_{j+1} can be expressed as a polynomial of degree $j+1$ in A_1. Since each ϕ_i is of degree i, we can express A^k as a linear combination of $\phi_0(A_1), ..., \phi_k(A_1)$. Therefore, $\{A^k : k = 0, ..., d\}$ is a basis for $\mathcal{A}$ and $\mathbb{C}[\mathcal{A}]$ is closed under matrix multiplication. Observing that

$$A_0 = I, \quad \sum_i A_i = J, \quad A_i^T = A_i,$$

we conclude that $\mathcal{A}$ is a P-polynomial association scheme. □

An immediate result of this Lemma 2.1.4 concerns continuous-time quantum walks on distance regular graphs. Recall that the unitary walk operator is defined as

$$U(t) = e^{-itA_1}.$$

The exponential can be expressed as a complex-valued polynomial in A_1, so $U(t) \in \mathcal{A}$. Therefore, the uv-entry of $U(t)$ depends only on the distance $d(u, v)$.

2.2 Semisimple Algebras

We will now introduce semisimple algebras. All of the results in this section are well-known; more detail can be found in [23] and [20].

Let $\mathcal{B}$ be a ring. We say that $\mathcal{B}$ is an *algebra* over the field $\mathbb{F}$ if there is a homomorphism ρ from $\mathbb{F}$ to the centre of $\mathcal{B}$. We will be dealing almost exclusively with algebras of complex-valued matrices. In this case, the homomorphism is given by

$$\rho(x) = xI$$

for all $x \in \mathbb{C}$. A *left ideal* of an algebra $\mathcal{B}$ is a subset $\mathcal{I}$ of $\mathcal{B}$ such that $\mathcal{B}\mathcal{I} \subseteq \mathcal{I}$. We say that an ideal is *minimal* if it properly contains no non-zero ideal.

Two idempotents e_1 and e_2 are orthogonal when

$$e_1 e_2 = e_2 e_1 = 0.$$

If e is an idempotent, then

$$e(1 - e) = e - e^2 = 0,$$

so $(1-e)$ is an orthogonal idempotent. An idempotent is *primitive* if it cannot be expressed as a sum of non-zero orthogonal idempotents. The following lemmas relate the idempotents and ideals of $\mathcal{B}$:

2.2.1 Lemma. *If e is an idempotent in $\mathcal{B}$ and $\mathcal{B}e$ is a minimal ideal, then e is primitive.*

Proof. Assume that $e = e_1 + e_2$ for orthogonal non-zero idempotents e_1 and e_2. Then, since $e_1e = e_1$ and $e_2e = e_2$, the ideals $\mathcal{B}e_1$ and $\mathcal{B}e_2$ are contained in $\mathcal{B}e$. Since $e_1 \in \mathcal{B}e_1$, this module is non-zero. However, $\mathcal{B}e_1e_2 = 0$, so $e_2 \notin \mathcal{B}e_1$. Since $e_2 \in \mathcal{B}e$, we must have $\mathcal{B}e_1 \subsetneq \mathcal{B}e$. So, if $\mathcal{B}e$ is minimal, then e is primitive. □

2.2.2 Lemma. *If $\mathcal{I}$ is a minimal left ideal such that $\mathcal{I}^2 \neq 0$, then there is some idempotent e in $\mathcal{B}$ such that $\mathcal{I} = \mathcal{B}e$.*

Proof. Let $\mathcal{I}$ be such an ideal. Since $\mathcal{I}^2 \neq 0$, there is some x in $\mathcal{I}$ such that $\mathcal{I}x \neq 0$. Since $\mathcal{I}x \subseteq \mathcal{I}$ and $\mathcal{I}$ is minimal, we must have $\mathcal{I}x = \mathcal{I}$. In particular, there must be some $e \in \mathcal{I}$ such that $ex = x$. As a consequence, $(e^2 - e)x = 0$. Let $\mathcal{C}$ be the ideal consisting of elements y of $\mathcal{I}$ such that $yx = 0$. Since $\mathcal{I}x \neq 0$, the ideal $\mathcal{C}$ is properly contained in $\mathcal{I}$. Since $\mathcal{I}$ is minimal, $\mathcal{C} = 0$. In particular, $(e^2 - e) = 0$ and e is an idempotent. Since $e \in \mathcal{I}$, we know that $\mathcal{B}e \subseteq \mathcal{I}$ and $\mathcal{B}e \neq 0$, so $\mathcal{B}e = \mathcal{I}$. □

Let M be a vector space over $\mathbb{F}$. Then, M is a $\mathcal{B}$-*module* if there is a homomorphism from $\mathcal{B}$ to $\mathrm{End}(M)$. In other words, a $\mathcal{B}$-module is an *invariant subspace*. Since the algebras we are concerned with will consist of complex-valued matrices, the homomorphism from $\mathcal{B}$ to $\mathrm{End}(M)$ is trivial—it is given by matrix multiplication. A *submodule* of M is a subspace of M that is also a $\mathcal{B}$-module. A *proper submodule* of M is one that is properly contained in M.

As an example, consider the action of $\mathcal{B}$ on itself. For each $a \in \mathcal{B}$, we can define an endomorphism ψ_a of $\mathcal{B}$:

$$\psi_a(b) = ab.$$

The action of these endomorphisms ψ_a on $\mathcal{B}$ defines the *regular module* of $\mathcal{B}$. The submodules of the regular module are the left ideals of $\mathcal{B}$.

A $\mathcal{B}$-module is *simple* if it has no non-zero proper submodules. A $\mathcal{B}$-module is *semisimple* if it can be expressed as a direct sum of simple modules. An algebra $\mathcal{B}$ is called a *semisimple algebra* if its regular module is semisimple. The following lemma highlights an important subset of semisimple algebras:

2.2.3 Lemma. *Let $\mathcal{B}$ be a finite dimensional matrix algebra over $\mathbb{C}$ equipped with an inner product. If $\mathcal{B}$ is closed under taking the adjoint relative to the inner product, then it is a semisimple algebra.*

Proof. If $\mathcal{B}$ has no proper submodules, then we are done. Otherwise, assume that M is a proper submodule of $\mathcal{B}$. We need only show that $M^{\perp}$ is also a $\mathcal{B}$-module. Take any x in $M^{\perp}$. Then, for any $a \in \mathcal{B}$ and any $y \in M$,

$$\langle y, ax \rangle = \langle a^* y, x \rangle = 0$$

since $a^* y \in M$. Therefore, $M^{\perp}$ is also a $\mathcal{B}$-module. Applying induction in the number of dimensions, we conclude that $\mathcal{B}$ is a semisimple algebra. □

Together with Lemmas 2.2.1 and 2.2.2, the following lemma relates simple modules, ideals and idempotents:

2.2.4 Lemma. *Let $\mathcal{B}$ be a semisimple algebra and M a simple $\mathcal{B}$-module. Then M is isomorphic to a simple submodule of $\mathcal{B}$.*

Proof. Let M be a non-zero simple $\mathcal{B}$-module. Since $\mathcal{B}$ is semisimple, it can be expressed as a direct sum of simple submodules. If, for each submodule $\mathcal{I}$ of $\mathcal{B}$, we have $\mathcal{I}M = 0$, then $\mathcal{B}M = 0$, a contradiction. Let $\mathcal{I}$ be a simple submodule of $\mathcal{B}$ such that $IM \neq 0$. Then, there is some $x \in M$ such that $Ix \neq 0$. But Ix is a submodule of M, we must have $Ix = M$.

The set of elements c of $\mathcal{I}$ such that $cx = 0$ is a submodule of $\mathcal{I}$. Since $\mathcal{I}x \neq 0$ and $\mathcal{I}$ is simple, we must have $c = 0$ whenever $cx = 0$. Now, take a, b in $\mathcal{I}$ such that $ax = bx$, and therefore $(a - b)x = 0$. Then $a = b$. Therefore, the map

$$a \mapsto ax$$

is a bijection between $\mathcal{I}$ and M that commutes with multiplication by $\mathcal{B}$, and M is isomorphic to $\mathcal{I}$. □

We have established the relationship between the minimal ideals of an algebra, its primitive idempotents, and its simple modules. In Chapter 5, we will study a semisimple algebra in the form of the Jaeger algebras. Our primary aim will be to identify and characterize the simple modules of these algebras. As we have seen, the characteristics of these modules tells us a good deal about the algebra itself.

Chapter 3

Quantum Walks

This chapter begins by defining the continuous time quantum walk. We then examine the phenomena of *periodicity*, *state transfer* and *strong cospectrality*. In Section 3.1.1, we define periodicity and outline some basic results. The material in this section is not new, but it will underpin a number of results in subsequent sections.

We begin Section 3.1.2, by defining perfect state transfer. Perfect state transfer refers to the transfer of amplitude between vertices in a quantum walk with perfect fidelity. We prove several new results concerning perfect state transfer. Theorem 3.1.14 gives strong conditions for perfect state transfer on G when the pairwise ratio of its eigenvalues is rational. We use this result in Theorem 3.1.15 and Corollary 3.1.16 to establish strong necessary conditions for perfect state transfer in bipartite graphs.

We then define pretty good state transfer; it is similar to perfect state transfer, but only requires fidelity arbitrarily close to one. Making use of a classical result of Kronecker, Theorem 3.1.19 states that pretty good state transfer occurs between u and v whenever the eigenvalue support of u and v satisfy certain linear independence conditions over the rationals. This is a new result. A variation of this result is applied in the joint work of the author, Godsil, Kirkland and Severini [28], concerning pretty good state transfer on the path. We review this result, which states that pretty good state transfer occurs between the endpoints of a path of length n if and only if $n + 1$ is a prime, twice a prime, or a power of two.

In Section 3.1.3, we examine strongly cospectral vertices in detail. Two vertices u and v are cospectral if $G \setminus u$ and $G \setminus v$ are cospectral. They are strongly cospectral if

$$E_r e_u = \pm E_r e_v$$

for all idempotents E_r of G. If there is perfect state transfer or pretty good state transfer between u and v, then they must be strongly copsectral. We prove several new results concerning pretty good state transfer. Theorem 3.1.12 gives a necessary and sufficient conditions for strong cospectrality in terms of the entries of the idempotents of G. Lemma 3.1.29 states that the number of vertices strongly cospectral to u cannot exceed the size of the eigenvalue support of u. Theorem 3.1.30 states that, if u and v are strongly cospectral, then there is a unitary matrix X that is a polynomial in A and swaps u and v. We make use of this in Theorem 3.1.32 and its corollary, which state that if G is a homogeneous graph, then X is an automorphism of G. Corollary 3.1.33 states that if G is distance regular, then the diameter of G is $d(u, v)$ and A_d is an automorphism of G. This is a surprisingly powerful implication of strong cospectrality. It leads us to wonder if a graph containing strongly cospectral vertices u and v always has an automorphism that swaps them. Theorem 3.1.34 provides a partial answer. It gives a method for constructing graphs with strongly cospectral pairs of vertices that are not contained in the same orbit.

In Section 3.2, we introduce multi-particle continuous time quantum walks. In a multi-particle walk, we allow for movement of the particles about the graph, as well as interaction among the particles. We establish a very general framework for these walks, requiring only that

(i) Movement of the particles should be governed by the structure of the graph

(ii) Interactions between a set of particles depends only on their pairwise distances in the graph.

This allows the results that we will prove in Chapter 4 to be as general as possible. We discuss Bosonic and Fermionic statistics as restrictions of multi-particle walks to the symmetric and anti-symmetric subspaces respectively. Finally, describe the k-Boson graph invariant, which was first introduced by Gamble, Friesen, Zhou, Joynt and Coppersmith [22]. The strength of this invariant will be examined in detail in Chapter 4.

Section 3.3 defines the discrete time quantum walk. We will then describe a graph invariant introduced by Emms, Hancock, Severini and Wilson [17].

If U is the unitary discrete-time walk operator, then the invariant of Emms et al. is the spectrum of the positive support of U^3. They conjecture that this invariant is strong enough to distinguish all strongly regular graphs. While the veracity of their conjecture remains an open question, we will establish some limitations on the strength of their invariant in Chapter 4.

3.1 Continuous Time Quantum Walks

The state of a continuous time quantum walk at time t is described by a complex column vector $\mathbf{x}(t)$, indexed by the vertices of the graph G. If we perform a measurement in the vertex basis, we get the result v with probability

$$\mathbf{x}_v(t)^* \mathbf{x}_v(t).$$

The evolution of the walk is determined by a Hermitian matrix H—our *Hamiltonian*. Since we would like our quantum walk to respect the structure of the graph G, our Hamiltonian should be derived from the structure of the graph. Unless otherwise stated, we will take the Hamiltonian to be the adjacency matrix A of G. The evolution of the walk is given by

$$i\frac{d}{dt}\mathbf{x}(t) = A\mathbf{x}(t).$$

Solving this equation yields

$$x(t) = e^{-iAt}\mathbf{x}(0).$$

Since A is Hermitian, $\exp(-iAt)$ is a unitary operator, which we call the *transition matrix*, and denote by $U(t)$. Note that

$$U(-t) = U(t)^{-1},$$

so the walk process is reversible. Since A is symmetric, $U(t)$ is also symmetric. Using the spectral decomposition of A, we can rewrite the adjacency matrix:

$$A = \sum_j p(j) E_j$$

where $\{E_j\}$ is a set of pairwise orthogonal idempotents, each of which can be expressed as a polynomial in A. Therefore, we can write the unitary walk operator as follows:

$$U(t) = \sum_j e^{-itp(j)} E_j.$$

As a consequence, for any t, the operator $U(t)$ is a polynomial in A.

We now consider the case when G is a distance regular graph, with adjacency matrix A_1. Recall that G defines an association scheme $\mathcal{A} = \mathcal{A}_G$. Since the transition matrix $U(t)$ is a polynomial in A_1, it is contained in $\mathcal{A}$. We can therefore express the transition matrix as a sum of basis relations of $\mathcal{A}$:

$$U(t) = \sum_k \sum_j e^{-itp_j(1)} q_j(k) A_k.$$

3.1.1 Periodicity

The evolution of a classical continuous time random walk is given by

$$\frac{d}{dt}\mathbf{p}(t) = L\mathbf{p}(t)$$

where $\mathbf{p}(t)$ is a vector of probabilities over the vertices of G and L is the *Laplacian*, defined by

$$L_{uv} = \begin{cases} 1 & uv \in E(G) \\ -\deg(u) & u = v \\ 0 & \text{otherwise.} \end{cases}$$

A classical random walk defined this way will always converge on a *stationary state*. A quantum walk does not have this property; in general, it does not approach an equilibrium state. As a result, it is natural to ask when a quantum walk returns to its starting state. If there is a time t and a complex number α such that

$$U(t)e_u = \alpha e_u,$$

then we say that the walk is *periodic* at u with phase α. If G is periodic at each vertex u at a single time t, then we say that G is periodic. The following results are proven by Godsil in [26] and [24].

3.1.1 Lemma. *If t_0 is the minimum positive time such that a quantum walk on G is periodic at t_0, then the walk is periodic at time t if and only if t is a multiple of t_0.*

Proof. Assume G is periodic at some time t greater than t_0 and not an integer multiple of t_0. Then, we can write

$$t = (a + b)t_0$$

where a is the largest integer such that $t_0 < t$ and $0 < b < 1$. In this case, the walk is periodic at time $bt_0 < t_0$, a contradiction. Therefore, t must be an integer multiple of t_0. The converse is trivial. □

We refer to the minimum value t_0 as the *period* of G.

3.1.2 Lemma. *If G is connected and periodic at time t, then there is some complex number α such that*

$$U(t) = \alpha I.$$

Proof. If the walk is periodic at t, then there is diagonal matrix D such that

$$U(t) = D.$$

Since $U(t)$ is a polynomial in A, we know that D commutes with A. Now, if u and v are adjacent, then

$$(DA)_{uv} = D_{uu}, \qquad (AD)_{uv} = D_{vv}.$$

Therefore, $D_{uu} = D_{vv}$ for all adjacent u, v. Since G is connected, $D = \alpha I$ for some α. □

In this case, we say that G is periodic at time t with phase α. We can identify the phase α by considering the spectral decomposition of A as follows:

3.1.3 Lemma. *If G is connected and periodic with period t_0 and phase α, then*

$$e^{-it_0 p(j)} = \alpha$$

for all eigenvalues $p(j)$.

Proof. Using the spectral decomposition,

$$\sum_j e^{-it_0 p(j)} E_j = \alpha I.$$

Since the E_j are linearly independent and

$$\sum_j E_j = I,$$

we have

$$e^{-it_0 p(j)} = \alpha$$

for all j. □

The following lemma will be particularly useful when applied to regular graphs:

3.1.4 Lemma. *If G is periodic and has a non-zero integer eigenvalue, then all of its eigenvalues are integers.*

Proof. If G has period t_0, then

$$U(t_0) = \alpha I$$

for some complex α. Then,

$$\det(U(t_0)) = \alpha^n$$

but

$$\det(e^{-iAt_0}) = e^{-it_0 \operatorname{tr}(A)} = 1$$

since $\operatorname{tr}(A) = 0$. Then,

$$e^{-int_0 p(j)} = 1$$

for all j and $nt_0 p(j)$ is a multiple of 2π. If $p(j)$ is an integer for some j, then nt_0 is a multiple of 2π and all of our eigenvalues are rational. Since the eigenvalues are also algebraic integers, they are integers. □

Therefore, if G is regular and periodic, it has integer eigenvalues. We will now state a partial converse to Lemma 3.1.4, First, we to need define the *greatest common divisor* of a set $\{x_i, ..., x_k\}$. If

$$\frac{x_i}{x_j} \in \mathbb{Q}$$

for all i and j, then greatest common divisor is the largest real number d such that

$$\frac{x_i}{d} \in \mathbb{Z}$$

for all i with $1 \leq i \leq k$. We denote this by

$$\text{GCD}\{x_1, ..., x_k\}.$$

Note that this is consistent with the usual notion of the greatest common divisor of a set of integers.

3.1.5 Lemma. *If G has eigenvalues $p(0),...,p(\ell)$ such that*

$$\frac{p(i)}{p(j)} \in \mathbb{Q}$$

for all i,j, then it is periodic with period $2\pi/d$, where

$$d = GCD\{p(j) - p(0) : j > 0\}. \qquad \square$$

Therefore, a regular graph is periodic if and only if it has integer eigenvalues. We now consider the case when G is periodic at a vertex u. The following result is referred to as the *ratio condition*. It is proven in [24]; similar results appear in [37] and [13]. Before stating the theorem, we define the *eigenvalue support* of a vertex u as the set of eigenvalues $p(r)$ with corresponding idempotents E_r such that

$$E_r e_u \neq 0.$$

3.1.6 Theorem. *Let G be a graph that is periodic at vertex u. Then, for any $p(i), p(j), p(k), p(l)$ in the eigenvalue support of u,*

$$\frac{p(i) - p(j)}{p(k) - p(\ell)} \in \mathbb{Q}.$$

Proof. Let S be the eigenvalue support of u. Then,

$$\{E_j e_u : \; p(j) \in S\}$$

is a set of linearly independent vectors that sum to e_u. Now, if G is periodic at u with period t_0 and phase α, then

$$\sum_{p(j)\in S} e^{-ip(j)t_0} E_j e_u = \alpha \sum_{p(j)\in S} E_j e_u.$$

Since the $E_j e_u$ are linearly independent, we have

$$e^{-ip(j)t_0} = \alpha$$

for all j with $p(j) \in S$. So, for any $p(i), p(j) \in S$, we have

$$t_0(p(i) - p(j)) = k\pi$$

for some integer k. $\square$

3.1.7 Corollary. *If G is periodic at u and the eigenvalue support of u contains two integers, then all of the values in the eigenvalue support of u are integers.* □

3.1.8 Corollary. *Let G be a bipartite graph that is periodic at u. If $p(i)$ and $p(k)$ are in the eigenvalue support of u, then*

$$\frac{p(i)}{p(k)} \in \mathbb{Q}.$$

Proof. Set $p(j) = -p(i)$ and $p(\ell) = -p(k)$ in Theorem 3.1.6. □

3.1.2 State Transfer

A graph G exhibits *perfect state transfer* from u to v if, for some time t,

$$U(t)e_u = \beta e_v.$$

Since $U(t)$ is symmetric, perfect state transfer from u to v implies perfect state transfer from v to u. The following lemma is presented in [25], and was originally proven by Kay:

3.1.9 Lemma. *If there is perfect state transfer from u to v and v to w, then $u = w$.*

Proof. Let t_{uv} be the smallest time at which perfect state transfer occurs from u to v, and t_{vw} the smallest time at which perfect state transfer occurs from v to w. Without loss of generality, assume that $t_{uv} < t_{vw}$. Then, there is perfect state transfer from w to u at time $t_{wu} = t_{vw} - t_{uv}$. As a result, there is perfect state transfer from v to w at time $t'_{vw} = |t_{uv} - t_{wu}|$. But $t'_{vw} < t_{vw}$, contradicting the assumption that t_{vw} is minimal. We conclude that $t_{vw} = t_{uv}$ and therefore $v = w$. □

The following lemma is due to Godsil, and is proven in [26]. It places a strong restriction on pairs of vertices exhibiting perfect state transfer.

3.1.10 Lemma. *If there is perfect state transfer from u to v, then*

$$E_j e_u = \pm E_j e_v$$

for all j.

Proof. We have
$$U(t)e_u = \beta e_v$$
and therefore
$$e^{-itp(j)}E_j e_u = \beta E_j e_v.$$
Rearranging,
$$\overline{\beta} e^{-itp(j)}E_j e_u = E_j e_v.$$
Since β and $e^{-itp(j)}$ are both complex numbers of norm one and E_j is a real-valued matrix,
$$E_j e_u = \pm E_j e_v.$$
□

We say that vertices u and v with
$$E_j e_u = \pm E_j e_v$$
for all j are *strongly cospectral*. We will explore the topic of strongly cospectral vertices in greater depth in Section 3.1.3.

The following easy lemma will prove useful in characterizing graphs with perfect state transfer:

3.1.11 Lemma. *If G has perfect state transfer from u to v at time t, then it is periodic at u with period $2t$.* □

In particular, if G is periodic with period t_0, then any perfect state transfer must occur at $t_0/2$.

3.1.12 Theorem. *Let u and v be vertices of G with identical eigenvalue support $p(0), ..., p(\ell)$. They are strongly cospectral if and only if there is a partition (Π^+, Π^-) of $\{0, ..., \ell\}$ such that*

(i) $\sum_{j\in\Pi^+}(E_j)_{uu} = \sum_{j\in\Pi^-}(E_j)_{uu} = \frac{1}{2}$

(ii) If $j \in \Pi^+$, then
$$E_j e_u = E_j e_v.$$
If $j \in \Pi^-$, then
$$E_j e_u = -E_j e_v.$$

Proof. Clearly, (ii) implies strong cospectrality, so we only need to prove that strong cospectrality implies (i) and (ii).

Define a vector σ such that

$$E_j e_u = \sigma_j E_j e_v.$$

Define

$$\Pi^+ = \{j : \sigma_j = 1\}, \qquad \Pi^- = \{j : \sigma_j = -1\}.$$

Then,

$$\sum_{j\in\Pi^+} (E_j)_{uu} + \sum_{j\in\Pi^-} (E_j)_{uu} = 1$$

while

$$\sum_{j\in\Pi^+} (E_j)_{uu} - \sum_{j\in\Pi^-} (E_j)_{uu} = 0.$$

So, (Π^+, Π^-) is a partition satisfying (i) and (ii). □

The following corollary concerns walk-regular graphs. A graph G with adjacency matrix A is *walk-regular* if, for any k, the diagonal entries of A^k are equal. The first is a corollary of Theorem 3.1.12:

3.1.13 Corollary. *Let G be a walk-regular graph with eigenvalues $p(0), .., p(\ell)$ and multiplicities $m_0, ..., m_\ell$. If G contains strongly cospectral vertices, then n is even and*

$$\sum_{j\in\Pi^+} m_j = \sum_{j\in\Pi^-} m_j = \frac{n}{2}.$$

Proof. This result is obtained by substituting $(E_j)_{uu} = \frac{m_j}{n}$ into Theorem 3.1.12. □

We will now apply Theorem 3.1.12 and its corollary to establish a necessary and sufficient condition for perfect state transfer.

3.1.14 Theorem. *Let u and v be vertices in a graph G. There is perfect state transfer from u to v if and only if the following conditions are met:*

(i) The vertices u and v have the same eigenvalue support $p(0), ..., p(\ell)$.

(ii) There is a partition (Π^+, Π^-) of the set $\{0, ..., \ell\}$ such that

- $\sum_{j\in\Pi^+} (E_j)_{uu} = \sum_{j\in\Pi^-} (E_j)_{uu} = \frac{1}{2}$

- *If $j \in \Pi^+$, then*
$$E_j e_u = E_j e_v.$$
If $j \in \Pi^-$, then
$$E_j e_u = -E_j e_v.$$

(iii) For all non-zero j, k, we have
$$\frac{p(j) - p(0)}{p(k) - p(0)} \in \mathbb{Q}$$
allowing us to define
$$d = \gcd\{p(j) - p(0) : \ j = 1, ..., \ell\}.$$
Then, for any $j \in \Pi^+$ and $k \in \Pi^-$,
$$p(j) \equiv p(k) + d \mod 2d.$$

If conditions (i)-(iii) are met, then perfect state transfer occurs at time π/d.

Proof. Assume that there is perfect state transfer from u to v. In this case, they are strongly cospectral, and must therefore have the same eigenvalue support, so (i) is required. Applying Theorem 3.1.12, we see that condition (ii) is necessary since u and v are strongly cospectral. We will now show that, if (i) and (ii) are true, condition (iii) is necessary and sufficient for perfect state transfer.

If there is perfect state transfer from u to v, the graph G is periodic at u and
$$\frac{p(j) - p(0)}{p(k) - p(0)} \in \mathbb{Q}$$
and we can define
$$d = \gcd\{p(j) - p(0) : \ j = 1, ..., \ell\}.$$
By Lemma 3.1.5, G has period $2\pi/d$ at u. Lemma 3.1.11 tells us that the perfect state transfer must occur at time π/d. This gives us
$$U(\pi/d)e_u = \sum_j e^{-i\pi p(j)/d} E_j e_u = \beta e_v.$$

We can rewrite this as

$$\begin{aligned}
0 &= \sum_j e^{-i\pi p(j)/d} E_j e_u - \beta e_v \\
&= \left(\sum_{j\in\Pi^+} e^{-i\pi p(j)/d} E_j - \sum_{k\in\Pi^-} e^{-i\pi p(k)/d} E_k - \beta I \right) e_v \\
&= \left(\sum_{j\in\Pi^+} (e^{-i\pi p(j)/d} - \beta) E_j - \sum_{k\in\Pi^-} (e^{-i\pi p(k)/d} + \beta) E_k \right) e_v .
\end{aligned}$$

Since the columns of $E_0, ..., E_\ell$ indexed by v are linearly independent, this means that

$$e^{-i\pi p(j)/d} = \begin{cases} \beta & j \in \Pi^+ \\ -\beta & j \in \Pi^-. \end{cases}$$

There is some value β for which this occurs if and only if

$$p(j) + d \equiv p(k) \mod 2d$$

for all $j \in \Pi^+$ and $k \in \Pi^-$. □

Theorem 3.1.14 gives us a straightforward procedure to check for perfect state transfer: calculate the spectral decomposition of A; partition $\{0, ..., \ell\}$ into Π^+ and Π^-; and verify that the eigenvalues satisfy the congruence identified in Theorem 3.1.14.

Example: Cocktail Party Graphs

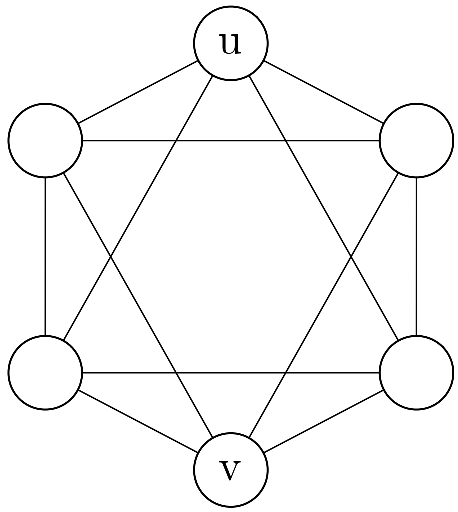
For an even positive integer n, the cocktail party graph $G_n = (V, E)$ can be defined as follows:

$$\begin{aligned}
V =& \mathbb{Z}_n \\
E =& \{(x, y) : \ x \neq y + n/2\}.
\end{aligned}$$

Figure 3.1.1 shows the cocktail party graph on 6 vertices. Set $u = 0$ and $v = n/2$. Then, u and v have shared eigenvalue support $\{-2, 0, n-2\}$. It is easily verified that u and v are strongly cospectral, with resulting partition of the eigenvalues

$$\Pi^+ = \{-2, n-2\}, \quad \Pi^- = \{0\}.$$

Figure 3.1.1: The cocktail party graph on 6 vertices.



This gives us

$$d = \gcd\{n, 2\} = 2.$$

So, there is perfect state transfer from u to v if and only if

$$n - 2 \equiv 2 \mod 4.$$

In other words, there is perfect state transfer if and only if n is divisible by 4.

Applying Theorem 3.1.14 to bipartite graphs, we get the following theorem:

3.1.15 Theorem. *Let G be a bipartite graph with perfect state transfer between vertices u and v in opposite sides of the bipartition of G. Then, for any $p(i), p(j), p(k)$ in the eigenvalue support of u,*

$$\frac{p(i)}{p(j) - p(k)} \notin \mathbb{Z}.$$

Proof. Assume that G is a bipartite graph with perfect state transfer between vertices u and v in opposite sides of the bipartition of G. Then, G is periodic at u and we can apply Corollary 3.1.8 and $p(i)/p(j)$ is rational for all i, j. We can now apply Theorem 3.1.14 to construct the partition (Π^+, Π^-) of the eigenvalue support of u. Since G is bipartite, if $p(i)$ is in the eigenvalue support of u, then there is some $p(i')$ in the eigenvalue support with $p(i') = -p(i)$. Moreover, since u and v are in opposite sides of the bipartition, i and i' are in opposite sides of the partition (Π^+, Π^-). Now, assume that

$$\frac{p(i)}{p(j) - p(k)} \in \mathbb{Z}$$

for some $p(j), p(k)$. Then, setting

$$d = \mathrm{GCD}\{p(j) - p(0) : j > 0\}$$

$(p(j) - p(k))/d$ must be an integer and therefore $p(i)/d$ must also be an integer. In this case,

$$p(i) \equiv p(i') \mod 2d.$$

Since i and i' are in opposite sides of the partition (Π^+, Π^-), this contradicts Theorem 3.1.14. We conclude that

$$\frac{p(i)}{p(j) - p(k)} \notin \mathbb{Z}$$

for all $p(i), p(j), p(k)$ in the eigenvalue support of u. □

3.1.16 Corollary. *Let G be a bipartite graph with u and v in opposite sides of the bipartition. If there is perfect state transfer from u to v, then zero is not in the eigenvalue support of u or v.* □

In 2003, Bose considered state transfer between the endpoints of the path [8]. His motivation was the physical transmission of a quantum state along a chain of coupled spins. He found that there was perfect state transfer for the path on two or three vertices, but there was never perfect state transfer for more than three vertices. We will now consider the case of general graphs where state transfer occurs with fidelity arbitrarily close to one—a phenomenon known as *pretty good state transfer*. We will ultimately return to the case of the path, providing necessary and sufficient conditions for pretty good state transfer in Theorem 3.1.21.

More formally, we say that a graph has *pretty good state transfer* from u to v if there is a complex number β with $|\beta| = 1$ and a sequence $\{t_j\}$ of real numbers such that

$$\lim_{j\to\infty} U(t_j)e_u = \gamma e_v.$$

In this case, we say that pretty good state transfer occurs with phase β. This definition is due to Godsil [25]. We will use t_δ to denote a time at which

$$|e_v^T U(t_\delta)e_u - \beta| < \delta.$$

The following Lemma, due to Godsil [26], shows that pretty good state transfer requires strong cospectrality:

3.1.17 Lemma. *If there is pretty good state transfer from u to v, then*

$$E_j e_u = \pm E_j e_v$$

for all j.

Proof. For any $\delta > 0$, there is some t_δ such that

$$U(t_\delta)e_u = \beta e_v + \epsilon$$

for some vector ϵ with $\|\epsilon\| < \delta$. Applying E_j to both sides and rearranging,

$$(\overline{\beta} e^{-it_\delta p(j)} e_u - E_j e_v) = \overline{\beta} E_j \epsilon.$$

Since the norm of the right side is at most δ, we can write

$$\lim_{\delta\to 0} \left(\overline{\beta} e^{-it_\delta p(j)} e_u\right) = E_j e_v$$

and define a complex number γ such that

$$\lim_{\delta\to 0} \left(\overline{\beta} e^{-it_\delta p(j)}\right) = \gamma.$$

We now have

$$\gamma E_j e_u = E_j e_v.$$

Since E_j is real-valued, this gives us

$$E_j e_u = \pm E_j e_v. \qquad \square$$

Note that this allows us to apply Theorem 3.1.12, giving us a strong necessary condition for pretty good state transfer on walk-regular graphs. We can rewrite the condition for pretty good state transfer as a set of approximate congruences, modulo 2π as follows:

$$\begin{aligned} t_\delta \cdot p(j) &\cong \gamma \mod (2\pi) \qquad j \in \Pi^+ \\ t_\delta \cdot p(j) &\cong \gamma + \pi \mod (2\pi) \qquad j \in \Pi^-. \end{aligned}$$

We will make use of the following theorem, due to Kronecker [33]. For a straightforward proof, see [9].

3.1.18 Theorem. *Let T^n be the n-dimensional torus:*

$$T^n = \frac{\mathbb{R}^n}{\mathbb{Z}^n}.$$

Then, the set

$$\frac{\mathbb{R}\mathbf{x}}{\mathbb{Z}^n}$$

generated by the real vector $\mathbf{x}$ is dense in T^n if and only if the entries of $\mathbf{x}$, along with 1, are linearly independent over the rational numbers. □

Therefore, if our eigenvalues are linearly independent, for any $\delta > 0$, we can find t_δ satisfying the congruences above to within δ. This gives us the following theorem:

3.1.19 Theorem. *Let G be a graph with strongly cospectral vertices u and v, and let $p(0), ..., p(\ell)$ be their eigenvalue support. If the set*

$$\{p(j) - p(0) : \ 1 \leq j \leq \ell\}$$

is linearly independent over the rationals, then there is pretty good state transfer from u to v. □

3.1.20 Corollary. *Let G be a bipartite graph with strongly cospectral vertices u and v. If the positive values in the eigenvalue support of u and v are linearly independent over the rationals, then there is pretty good state transfer from u to v.* □

We will now apply this corollary to determine when pretty good state transfer takes place between the endpoints the path on n vertices.

Example: Pretty Good State Transfer on Paths

Bose [8] proved that there is perfect state transfer between the endpoints of a path if and only if it is the path on two or three vertices. We will now examine pretty good state transfer on paths of various lengths. We will first show that pretty good state transfer can occur with a restricted set of phases, depending on the length of the path. We will then prove the following theorem, the result of joint work of the author, Godsil, Severini and Kirkland [28]:

3.1.21 Theorem. *Pretty good state transfer occurs between the endpoints of a path of length n if and only if*

(i) $n = 2^r - 1$ *for some integer* r*;*

(ii) $n = p - 1$ *for prime* p*; or*

(iii) $n = 2p - 1$ *for prime* p*.*

Let P_n denote the path on n vertices, labeled $1, ..., n$. The eigenvalues of P_n are

$$p(j) = 2\cos\left(\frac{j\pi}{n+1}\right)$$

with corresponding eigenvectors $\mathbf{x}^1, ..., \mathbf{x}^n$ where

$$\mathbf{x}_v^j = \sin\left(\frac{jv\pi}{n+1}\right).$$

Letting $u = n - v + 1$, we observe that

$$\mathbf{x}_u^j = (-1)^{j-1}\mathbf{x}_v^j.$$

Therefore, u and v are strongly cospectral and the partition (Π^+, Π^-) of Theorem 3.1.12 separates $\{1, ..., n\}$ into odd and even subsets. We also note that

$$p(j) = -p(n - j + 1).$$

Let T be the permutation matrix that swaps u and $n-u+1$ for all u. Then,

$$T = -\sum_{j=1}^{n}(-1)^j E_j.$$

Now, if there is pretty good state transfer from u to v with phase β, then

$$\beta T \approx U(t_\delta).$$

Equivalently,

$$-\beta \sum_{j=1}^{n} (-1)^j E_j \approx \sum_{j=1}^{n} e^{-it_\delta p(j)} E_j.$$

We can use this to prove the following lemma:

3.1.22 Lemma. *If there is pretty good state transfer from u to v in with phase β in P_n, then*

- *If n is even, then $\beta = \pm i$.*
- *If $n \equiv 1 \mod 4$, then $\beta = 1$.*
- *If $n \equiv 3 \mod 4$, then $\beta = -1$.*

Proof. If n is even, then one of $\{j, n-j+1\}$ is in Π^+, while the other is in Π^-, so

$$e^{-it_\delta p(j)} \approx -e^{-it_\delta p(n-j+1)} = -e^{it_\delta p(j)}$$

and $\beta = \pm i$. On the other hand, if n is odd, then j and $n-j+1$ are both in Π^+ or both in Π^-, so

$$e^{-it_\delta p(j)} \approx e^{-it_\delta p(n-j+1)} = e^{it_\delta p(j)}$$

and $\beta = \pm 1$. Now, note that

$$\det(e^{-it_\delta A}) = e^{-it_\delta \operatorname{tr}(A)}) = 1$$

Since $\operatorname{tr}(A) = 0$. We can also calculate

$$\det(e^{-it_\delta A}) \approx (-1)^{\lfloor n/2 \rfloor} \beta^n.$$

Solving gives us $\beta = 1$ when $n \equiv 1$ and $\beta = -1$ when $n \equiv 3$ modulo 4. □

3.1.23 Corollary. *For appropriate β, as identified in Lemma 3.1.22,*

$$e^{-it_\delta p(j)} \approx (-1)^{j-1}\beta$$

if and only if

$$e^{-it_\delta p(n-j+1)} \approx (-1)^{n-j}\beta. \qquad \square$$

As a result of this Corollary, we need only consider $j = 1, ..., \lfloor n/2 \rfloor$. That is, if $p(1), ..., p(\lfloor n/2 \rfloor)$ are linearly independent over the rationals, then there is pretty good state transfer on the path of length n. We make use of the following result of Watkins and Zeitlin [39]:

3.1.24 Theorem. *Let $\psi(x)$ be the minimal polynomial of $\cos(\pi/m)$ over the rationals. Then,*

$$\deg(\psi(x)) = \begin{cases} \phi(m)/2 & m \text{ odd} \\ \phi(m) & m \text{ even} \end{cases}$$

where ϕ is the Euler totient function. $\square$

3.1.25 Lemma. *The eigenvalue*

$$p(j) = 2\cos\left(\frac{j\pi}{n+1}\right)$$

can be expressed as a polynomial in

$$p(1) = 2\cos\left(\frac{\pi}{n+1}\right)$$

with rational coefficients and degree at most j.

Proof. The following relation is easily proven:

$$\cos\left(\frac{j\pi}{n+1}\right) = 2\cos\left(\frac{\pi}{n+1}\right)\cos\left(\frac{(j-1)\pi}{n+1}\right) - \cos\left(\frac{(j-2)\pi}{n+1}\right).$$

As a result, if we define $p(0) = 1$, then

$$p(j) = p(1)p(j-1) - p(j-2)$$

and the lemma follows immediately. $\square$

Combining the Theorem 3.1.24 and Lemma 3.1.25, the eigenvalues

$$p(1), ..., p(\lfloor n/2 \rfloor)$$

are linearly independent over the rationals if

$$\frac{\phi(n+1)}{2} \geq \lfloor n/2 \rfloor$$

for n even, or

$$\phi(n+1) \geq \lfloor n/2 \rfloor$$

for n odd. Verifying that

$$\phi(2^r) = 2^{r-1}, \qquad \phi(2p) = p-1, \qquad \phi(p) = p-1,$$

we conclude that the conditions of Theorem 3.1.21 are sufficient.

Now, assume that $n+1 = rs$, where r is odd and $s \geq 3$. Note that this is the case if and only if n does not meet any of the conditions of Theorem 3.1.21. We now make use of the following identity:

$$1 + 2\sum_{j=1}^{\frac{r-1}{2}} (-1)^j \cos\left(\frac{j\pi}{r}\right) = 0.$$

Multiplying this by $\cos(\pi/(n+1))$ and $\cos(2\pi/(n+1))$ respectively yields

$$\begin{aligned}
\cos\left(\frac{\pi}{n+1}\right) + \sum_{j=1}^{\frac{r-1}{2}} (-1)^j \left[\cos\left(\frac{(sj+1)\pi}{n+1}\right) + \cos\left(\frac{(sj-1)\pi}{n+1}\right)\right] &= 0 \\
\cos\left(\frac{2\pi}{n+1}\right) + \sum_{j=1}^{\frac{r-1}{2}} (-1)^j \left[\cos\left(\frac{(sj+2)\pi}{n+1}\right) + \cos\left(\frac{(sj-2)\pi}{n+1}\right)\right] &= 0.
\end{aligned}$$

Subtracting the second equation from the first and multiplying by 2 yields

$$p(1) - p(2) + \sum_{j=1}^{\frac{r-1}{2}} (-1)^j \left(p(rj+1) - p(rj+2) + p(rj-1) - p(rj-2)\right) = 0.$$

Let L denote the left side of this equation. Exponentiating gives us

$$e^{itL} = 1$$

for all t. Now, note that

$$e^{it_\delta(p(j)-p(j+1))} \approx -1$$

for all j, so

$$e^{it_\delta(p(j+1)-p(j+2))} \cdot e^{it_\delta(p(j-1)-p(j-2))} \approx 1.$$

Substituting this into the expression for $e^{it_\delta L}$ gives

$$e^{it_\delta L} \approx -1$$

contradicting the fact that $e^{itL} = 1$. Therefore, the conditions of Theorem 3.1.21 are necessary as well as sufficient.

The most interesting consequence of this result is that identifying pretty good state transfer in paths of even length is equivalent to testing for primality. If P_n is a path of even length that does not exhibit pretty good state transfer, then there is some value $\epsilon(n) < 1$ such that

$$|e_n U(t) e_1| \leq \epsilon(n).$$

If we can efficiently calculate the value $\epsilon(n)$ as a function of n, then providing a time t for which

$$|e_n U(t) e_1| > \epsilon(n)$$

gives a certificate for the primality of $n+1$. Of course, such a certificate t might be arbitrarily long; placing a bound on the size of t is therefore of great interest as well.

3.1.3 Strongly Cospectral Vertices

The *characteristic polynomial* $\phi(G,t)$ of a graph G is defined by

$$\phi(G,t) = \det(tI - A)$$

where A is the adjacency matrix of G. The roots of the characteristic polynomial are the eigenvalues of G. The *walk generating function* $W(G,t)$ is given by

$$W(G,t) = \sum_{j=0}^{\infty} (At)^j.$$

Note that we can also express the walk generating function as follows:

$$W(G,t) = (I - tA)^{-1}.$$

Two vertices u and v of G are *cospectral* if

$$\phi(G \setminus u) = \phi(G \setminus v).$$

We will make use of the following lemma, which allows us to recast cospectrality in terms of the walk generating function. The proof is due to Godsil and Royle [29].

3.1.26 Lemma. *Take any vertex u in G. Then,*

$$\frac{\phi(G \setminus u, t)}{\phi(G,t)} = (tI - A)^{-1}_{uu}.$$

Proof. The uu entry of $(tI - A)^{-1}$ is given by

$$(tI - A)^{-1}_{uu} = \frac{(\mathrm{adj}(tI - A))_{uu}}{\det(tI - A)} = \frac{(\mathrm{adj}(tI - A))_{uu}}{\phi(G,t)}$$

where adj() denotes the adjugate matrix. The uu entry of the adjugate is the determinant of the matrix obtained by removing row u and column u. That is, it is the characteristic polynomial $\phi(G \setminus u, t)$. □

3.1.27 Corollary. *The vertices u and v are cospectral if and only if*

$$W(G,t)_{uu} = W(G,t)_{vv}.$$ □

3.1.28 Corollary. *The vertices u and v are cospectral if and only if*

$$(E_r)_{uu} = (E_r)_{vv}$$

for each idempotent E_r of G. □

Recall that two vertices, u and v in a graph G are *strongly cospectral* if

$$E_r e_u = \pm E_r e_v$$

for all idempotents E_r associated with G. Since each E_r is symmetric, this implies

$$(E_r)_{uu} = (E_r)_{vv}$$

so strongly cospectral vertices are cospectral. Lemma 3.1.17 shows that if there is pretty good state transfer from u to v, then they must be strongly cospectral. We note that the converse is not true in general; we have already seen that the endpoints of a path of length n are strongly cospectral, but do not exhibit pretty good state transfer when $n+1$ is not a prime, twice a prime, or a power of two. We begin by repeating Theorem 3.1.12,which places conditions on the idempotents of a graph G containing strongly cospectral vertices:

Theorem 3.1.12. *Let G be a graph with idempotents $E_0, ..., E_\ell$. Then, vertices u and v are strongly cospectral if and only if there is a partition (Π^+, Π^-) of $\{0, ..., \ell\}$ such that*

(i) $\sum_{j\in\Pi^+}(E_j)_{uu} = \sum_{j\in\Pi^-}(E_j)_{uu} = \frac{1}{2}$

(ii) If $j \in \Pi^+$, then

$$E_j e_u = E_j e_v.$$

If $j \in \Pi^-$, then

$$E_j e_u = -E_j e_v.$$

□

We will now state several new results, culminating with Theorem 3.1.34. The following lemma limits the size of a set of pairwise strongly cospectral vertices:

3.1.29 Lemma. *Let q be the size of the eigenvalue support of a vertex v_0. Then, there are at most $q-1$ other vertices that are strongly cospectral to u.*

Proof. Let $v_1, ..., v_\ell$ be the set of vertices other than v_0 that are strongly cospectral with v_0. Define a series of ± 1-vectors $\sigma^0, ..., \sigma^\ell$ such that

$$E_r e_{v_0} = \sigma^s_r \cdot E_r e_{v_s}.$$

Let M be a matrix with r^{th} column equal to $E_r e_{v_0}$. Then, since

$$\sum_r E_r = I,$$

we have

$$M\sigma^k = e_{v_k}.$$

The number of non-zero columns in M is equal to the size of the eigenvalue support of v_0. Therefore, the number of vertices cospectral to v_0 is bounded above by the size of the eigenvalue support of v_0. □

An interesting open question concerns the exact relationship between the set of vertices strongly cospectral to u and the orbit of u. A reasonable conjecture would be that, if u and v are strongly cospectral, then there is an automorphism that swaps u and v. While this conjecture proves to be false, we show that, if u and v are strongly cospectral, then there is a symmetric orthogonal matrix that commutes with A and swaps u and v:

3.1.30 Lemma. *Let u and v be strongly cospectral vertices in a graph G with adjacency matrix A. Then, there is a matrix X with eigenvalues ± 1 that is a polynomial in A and*

$$Xe_u = e_v, \qquad Xe_v = e_u.$$

Proof. As in the proof of Lemma 3.1.29, define a vector σ such that

$$E_r e_u = \sigma_r E_r e_v.$$

Recall that we can write

$$A = \sum_r p(r) E_r$$

where the E_r are idempotents and can be expressed as polynomials in A. Now, define the matrix X as follows:

$$X = \sum_r \sigma_r E_r.$$

Then, X is a symmetric, real-valued matrix such that

$$Xe_u = e_v, \qquad Xe_v = e_u, \qquad X^2 = I.$$

Therefore, X is the required unitary matrix. □

The following related lemma applies to all cospectral pairs of vertices. Rather than X being polynomial in A, we can only show that it commutes with A.

3.1.31 Lemma. *If u and v are cospectral vertices of G, then there is a matrix X with eigenvalues ± 1 that X commutes with A and*

$$Xe_u = e_v, \qquad Xe_v = e_u.$$

Proof. Although this result is new, the approach and terminology are due to Godsil ([26], Chapter 14). Let U^+ and U^- denote the cyclic A-modules generated by $(e_u + e_v)$ and $(e_u - e_v)$ respectively. Then, for any idempotent E_r,

$$(e_u - e_v)E_r(e_u + e_v) = (E_r)_{uu} - (E_r)_{vv} = 0$$

when u and v are cospectral. Therefore, U^+ and U^- are orthogonal. Let U^0 denote the orthogonal complement of the sum of U^+ and U^-. Then, U^0 consists of vectors $\mathbf{z}$ with $\mathbf{z}_u = \mathbf{z}_v = 0$. We can choose an orthonormal set of eigenvectors $\mathcal{E}$ of G such that each eigenvector lies in exactly one of U^+, U^- or U^0. Let

$$\begin{aligned} \mathcal{E}^+ =& \mathcal{E} \cap U^+ \\ \mathcal{E}^- =& \mathcal{E} \cap U^-. \end{aligned}$$

Then, setting

$$X = \sum_{\mathbf{x} \in \mathcal{E}^+} \mathbf{x}\mathbf{x}^T - \sum_{\mathbf{y} \in \mathcal{E}^-} \mathbf{y}\mathbf{y}^T$$

completes the proof. □

Clearly, if there is an automorphism of G that swaps u and v, then they are strongly cospectral. It is natural to ask if the converse holds. The following lemma answers the question for homogeneous graphs, which are defined in Section 4.1. In particular, this class of graphs contains all distance regular graphs.

3.1.32 Theorem. *Let G be a homogeneous graph with strongly cospectral vertices u and v. Then there is an automorphism P of G that swaps u and v. Moreover, $P = p(A)$ for some polynomial p.*

Proof. By Lemma 3.1.30, we know that there is a matrix X that is a expressible as a polynomial in A and

$$Xe_u = e_v, \qquad Xe_v = e_u.$$

Let $\mathcal{A}$ be the smallest association scheme containing A. Then, $X \in \mathcal{A}$. Since row u of X has a single 1, and the rest of its entries are 0, X must be a basis relation of $\mathcal{A}$. Each row and column therefore contains exactly one 1. That is, X is a symmetric permutation matrix that commutes with A. It therefore gives an automorphism of G which swaps u and v. □

3.1.33 Corollary. *Let G be a distance regular graph with strongly cospectral vertices u and v at distance d. Then*

(i) the diameter of G is d

(ii) u is the unique vertex that is strongly cospectral with v

(iii) u is the unique vertex at distance d from v

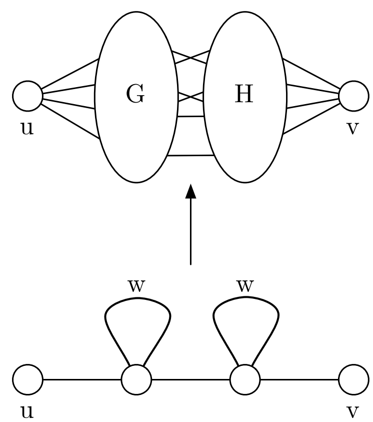
(iv) the distance d adjacency matrix A_d is an automorphism of G with $A_d^2 = I$.

Proof. Theorem 3.1.32 tells us that there is an automorphism $P = p(A)$ that swaps u and v with $P^2 = I$. Then, P is contained in $\mathcal{A}$, the association scheme of G. If $d = d(u, v)$, then the support of P includes A_d. Since P is a 01-matrix with rows summing to one, we must have $P = A_d$. Then u is the unique vertex at distance d from v. If the diameter of G is greater than d, then v is a cut vertex; this contradicts the fact that G is distance regular. □

We have seen that if G is a homogeneous graph with strongly cospectral vertices u and v, then there must be an automorphism swapping u and v. This leads us to wonder if such an automorphism always exists for strongly cospectral u and v. Bachman et al. have demonstrated that there are graphs with perfect state transfer between u and v that do not admit an automorphism swapping them [28, 26, 6]. Their construction takes a weighted looped path on four vertices and lifts it to a glued double-cone graph. It is illustrated in Figure 3.1.2. The weight w is chosen so that perfect state transfer occurs in the weighted path. G and H are non-isomorphic k-regular graphs, where k is a function of w. This construction relies on the fact that the path is a quotient of the glued double cone. The construction of Bachman et al., though interesting, provides a narrow class of counter-examples. There are no bipartite graphs among their constructions, for example. In the following theorem, we construct graphs with strongly cospectral vertices u and v and no automorphism swapping u and v. These graphs do not rely on having a weighted path as a quotient.

3.1.34 Theorem. *Let $G = (V, E)$ be a graph with cospectral vertices u and v. Let $H = (V', E')$ be the graph constructed by taking two identical copies*

Figure 3.1.2: The construction of Bachman et al..



of G, and joining the vertex u of one copy to the vertex v of the other:

$$\begin{aligned} V' =& V \times \{0,1\} \\ E' =& \{((x,i),(y,i)) : xy \in E, i \in \{0,1\}\} \\ & \cup \{((u,0),(v,1))\} \end{aligned}$$

Then, $(u,0)$ and $(v,1)$ are strongly cospectral.

This construction is illustrated in Figure 3.1.3. Before we prove this theorem, we need several lemmas. Let G_u^w denote the graph obtained from G by adding a loop on the vertex u with weight w.For convenience, we will use G_u^+ and G_u^- to denote the case where the weight is $+1$ and -1 respectively.

3.1.35 Lemma. *Let G_u^w be the graph obtained by adding a loop with weight w on vertex u. If $\phi(G,t)$ is the characteristic polynomial of G, then*

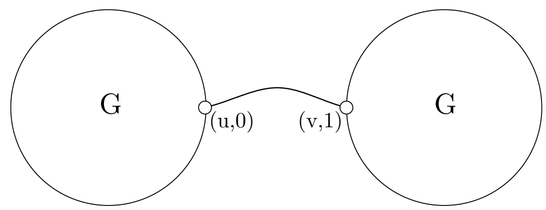
$$\phi(G_u^w) = \phi(G,t) + w \cdot \phi(G \setminus u, t).$$

Proof. This is a direct consequence of the expression for the characteristic polynomial

$$\phi(G,t) = \det(A - tI)$$

along with the definition of the determinant. □

Figure 3.1.3: The graph H of Theorem 3.1.34 is constructed by joining two copies of G.



As a result, if u and v are cospectral vertices, then G_u^w and G_v^w are cospectral graphs. Additionally, if θ is a root of any two of

$$\{\phi(G_u^+, t), \phi(G_u^-, t), \phi(G, t), \phi(G \setminus u, t)\}$$

then it is a root of all of them. The next lemma describes the eigenvalues of G_u^+ that are not eigenvalues of G:

3.1.36 Lemma. *The rational functions*

$$\frac{\phi(G,t)}{\phi(G_u^+,t)}, \quad \frac{\phi(G,t)}{\phi(G_u^-,t)}$$

of t have only simple poles. Moreover, these poles occur exactly at the eigenvalues G_u^+ in the eigenvalue support of u.

Proof. We have

$$\begin{aligned}\frac{\phi(G,t)}{\phi(G_u^+,t)} &= 1 + \frac{\phi(G \setminus u,t)}{\phi(G_u^+,t)} \\ &= 1 + (tI - A(G_u^+))_{uu}^{-1} \\ &= 1 + \sum_r \frac{(E_r)_{uu}}{t-\theta_r}.\end{aligned}$$

An analogous argument gives the result for G_u^-. □

3.1.37 Corollary. *Let G be a graph with cospectral vertices u and v. If θ_r is an eigenvalue of G_u^+ with corresponding idempotent E_r, then either* *(i)* θ_r *is also an eigenvalue of* G, G_u^- *and* G_v^+. *Therefore,*

$$(E_r)_{uu} = (E_r)_{vv} = 0.$$

(ii) θ_r *is not an eigenvalue of* G, *and is therefore not an eigenvalue of* G_u^- *nor* G_v^-. *In this case,* θ_r *is a simple eigenvalue with* $(E_r)_{uu} \neq 0$.

We will now use these results to construct a set of eigenvectors for the graph H of Theorem 3.1.34. Define $\mathcal{E}_u^+$ to be the set of eigenvectors $\mathbf{x}$ of G_u^+ with eigenvalue $\theta(\mathbf{x})$ such that $\theta(\mathbf{x})$ is not an eigenvalue of G. For convenience, we scale each $\mathbf{x}$ in $\mathcal{E}_u^+$ so that $\mathbf{x}_u = 1$; note that this is possible by Corollary 3.1.37. Define the sets $\mathcal{E}_u^-, \mathcal{E}_v^+$ and $\mathcal{E}_v^-$ analogously. Finally, let $\mathcal{E}_u^0$ be the set of eigenvectors $\mathbf{x}$ of G_u^+ that are also eigenvectors of G. These are also eigenvectors of G_u^-, G_v^+ and G_v^- and satisfy $\mathbf{x}_u = \mathbf{x}_v = 0$. For convenience, we stipulate that $\mathcal{E}_u^0$ is orthonormal.

Now, let $\mathbf{x} \oplus \mathbf{y}$ denote the vector indexed by the vertices of H that is constructed by assigning $\mathbf{x}$ to the left copy of G and $\mathbf{y}$ to the right copy. More formally,

$$(\mathbf{x} \oplus \mathbf{y})_{(u,i)} = \begin{cases} \mathbf{x}_u & i = 0 \\ \mathbf{y}_u & i = 1. \end{cases}$$

Define

$$\mathcal{E}^+ = \{\mathbf{x} \oplus \mathbf{y} :\ \mathbf{x} \in \mathcal{E}_u^+,\ \mathbf{y} \in \mathcal{E}_v^+,\ \theta(\mathbf{x}) = \theta(\mathbf{y})\}.$$

Then, each $\mathbf{x} \oplus \mathbf{y}$ in $\mathcal{E}^+$ is an eigenvector of H with eigenvalue $\theta(\mathbf{x})$. Moreover, $\theta(\mathbf{x})$ is a simple eigenvalue. Similarly, define

$$\mathcal{E}^- = \{\mathbf{x} \oplus (-\mathbf{y}) :\ \mathbf{x} \in \mathcal{E}_u^-,\ \mathbf{y} \in \mathcal{E}_v^-,\ \theta(\mathbf{x}) = \theta(\mathbf{y})\}.$$

Finally, set

$$\mathcal{E}^0 = \{\mathbf{x} \oplus \mathbf{x} :\ \mathbf{x} \in \mathcal{E}_u^0\} \cup \{\mathbf{x} \oplus (-\mathbf{x}) :\ \mathbf{x} \in \mathcal{E}_u^0\}$$

and

$$\mathcal{E} = \mathcal{E}^+ \cup \mathcal{E}^- \cup \mathcal{E}^0.$$

Then, $\mathcal{E}$ is a set of orthogonal eigenvectors of H. For each $\mathbf{z}$ in $\mathcal{E}$, one of the following holds:

(i) $\theta(\mathbf{z})$ is an eigenvalue of G as well as H and

$$\mathbf{z}_u = \mathbf{z}_v = 0.$$

(ii) $\theta(\mathbf{z})$ is a simple eigenvalue of H and

$$\mathbf{z}_u = \pm\mathbf{z}_v.$$

Therefore, $(u, 0)$ and $(v, 1)$ are strongly cospectral in H. □

The proof of Theorem 3.1.34 also serves as a constructive proof of the following well-known expression for $\phi(H)$:

$$\begin{aligned}\phi(H,t) =&\phi(G_u^+,t)\phi(G_v^-,t)\\ =&\left(\phi(G,t)+\phi(G\setminus u,t)\right)\left(\phi(G,t)-\phi(G\setminus u,t)\right)\\ =&\phi(G,t)^2-\phi(G\setminus u,t)^2\end{aligned}$$

Theorem 3.1.34 can also be proven by making use of the following result of Godsil [26]:

3.1.38 Theorem. *The vertices u and v of G are strongly cospectral if and only if they are cospectral and the rational function*

$$\frac{\phi(G\setminus\{u,v\},t)}{\phi(G,t)}$$

has only simple poles. □

In our case, this rational function is given by

$$\begin{aligned}\frac{\phi(G\setminus\{u,v\},t)}{\phi(G,t)} =&\frac{\phi(G\setminus u,t)^2}{\phi(G_u^+,t)\phi(G_u^-,t)}\\ =&\frac{\phi(G\setminus u,t)}{\phi(G_u^+,t)}\cdot\frac{\phi(G\setminus u,t)}{\phi(G_u^-,t)}\end{aligned}$$

Now, if θ is a root of $\phi(G_u^+,t)$ with multiplicity r and a root of $\phi(G_u^-,t)$ with multiplicity s, then it is a root of $\phi(G\setminus u,t)$ with multiplicity at least $\min\{r,s\}$. Therefore, we need only consider when one of

$$\frac{\phi(G\setminus u,t)}{\phi(G_u^+,t)},\quad \frac{\phi(G\setminus u,t)}{\phi(G_u^-,t)}$$

has non-simple poles. However,

$$\begin{aligned}\frac{\phi(G\setminus u,t)}{\phi(G_u^+,t)} =&(tI-A(G_u^+))^{-1}_{uu}\\ =&\sum_r\frac{(E_r)_{uu}}{t-\theta_r}.\end{aligned}$$

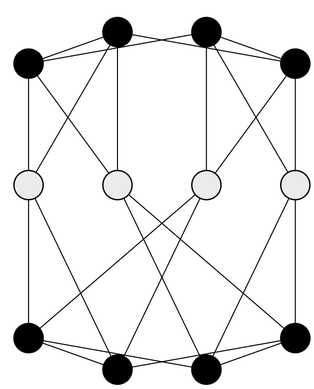
Applying the same argument for G_u^-, we see that neither expression has non-simple poles and u and v are strongly cospectral. This concludes the proof of Theorem 3.1.34.

Take a graph G with cospectral vertices u and v such that u and v are not in the same orbit. Then, constructing H as in Theorem 3.1.34 gives us a graph with a strongly cospectral pair of vertices u' and v' such that no automorphism of H swaps u' and v'. In fact, u' and v' are not in the same orbit in G'. Iterating this process yields graphs of this type of arbitrarily large size. If we begin with a tree T, then this process yields a sequence of trees with strongly cospectral vertices that are not swapped by any automorphism. Indeed, many families of graphs are closed under this simple operation.

Example: Strongly Cospectral Vertices in Disjoint Orbits

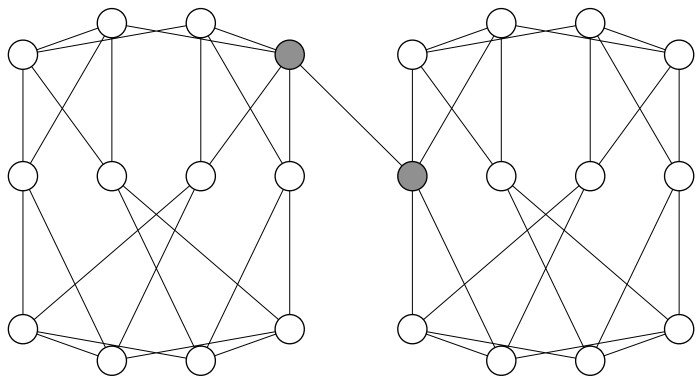
We now present an application of Theorem 3.1.34. We begin with the graph G, pictured in Figure 3.1.4. This graph is walk regular but not vertex transitive; its orbits have been highlighted in the figure. Since it is walk-regular, every pair of vertices is cospectral.

Figure 3.1.4: A walk regular graph G that is not vertex transitive. The orbits are highlighted.



It is easily verified through computation that no pair of vertices in G is strongly cospectral. Therefore, applying the construction of Theorem 3.1.34 yields a pair of strongly cospectral vertices that are in distinct orbits in G'. This is illustrated in Figure 3.1.5.

Figure 3.1.5: The graph G'. The highlighted vertices are strongly cospectral, but lie in distinct orbits of G'.



3.2 Multi-Particle Quantum Walks

The state space of a k-particle quantum walk consists of complex unit vectors indexed by V^k:

$$\mathbf{x} = (x_1, ..., x_k).$$

Here, x_j indicates the position of the j^{th} particle. The evolution of this walk will be determined by a Hamiltonian consisting of a movement term M and an interaction term N:

$$H = M + N.$$

We place two restrictions on the Hamiltonian:

(i) Movement of the particles should be governed by the structure of the graph.

(ii) Interactions among a set of particles is based only on their pairwise distances in the graph.

We consider a very general movement term

$$M = \sum_i a_i M_i$$

where M_i is a tensor product of copies of A and I. Taking movement terms of this form gives us a good deal of latitude, while still requiring that the movement of the particles be governed by the structure of the graph.

We now consider the interaction term N. Let D be an $k \times k$ matrix of non-negative integers with zero on the diagonal. Define the relation Δ_D such that

$$(\Delta_D)_{x,y} = \begin{cases} 1 & d(x_i, y_j) = D_{ij} \text{ for all } i, j \\ 0 & \text{otherwise.} \end{cases}$$

We can then write our interaction term as

$$N = -\sum_j b_j \Delta_{D_j}$$

for symmetric $n \times n$ matrices D_j with non-negative entries and zero on the diagonal. Note that the zeros on the diagonal ensure that each Δ_{D_j} acts as the identity on a subset of k-particle states. Thus, the interaction term applies an energy penalty based on the pairwise distances of the particles.

Typically, we consider Hamiltonians that do not depend on the order of the particles. That is, both the movement and interaction operators must commute with the permutation of the k particles. Specifically, the most common choice for the movement operator is

$$M = A^{\oplus k} = (A \otimes \overbrace{I \otimes ... \otimes I}^{k-1}) + (I \otimes A \otimes \overbrace{I \otimes ... \otimes I}^{k-2}) + ... + (\overbrace{I \otimes ... \otimes I}^{k-1} \otimes A).$$

This allows each of the k particles moving independently. Note that $A^{\oplus k}$ is also the adjacency matrix of the k^{th} Cartesian power of the graph G. It is also common to consider only *local* interactions between pairs of particles. That is, our interaction term contributes an energy penalty b for each distinct pair of particles located at the same vertex. Let $\chi(i, j)$ be an indicator variable that takes the value 1 when particles i and j are in the same location. Then, we define the interaction term N as follows:

$$\mathbf{y}^T N \mathbf{x} = \begin{cases} \frac{-b}{2} \sum_{i \neq j} \chi(i, j) & \mathbf{x} = \mathbf{y} \\ 0 & \text{otherwise.} \end{cases}$$

We will refer to this as the *local interaction term* and denote it by N_L. The local interaction term is independent of the order of the particles, and therefore commutes with permutation of the particles. For a matrix D, let $\mu(D)$ denote the number of zeros in non-diagonal entries of D. Then, letting $\mathcal{D}$ be the set of all symmetric $n \times n$ matrices with zero on the diagonal, we can express N_L as a sum of Δ_D terms as follows:

$$N = \frac{-b}{2} \sum_{D \in \mathcal{D}} \mu(D) \Delta_D.$$

Setting

$$H = A^{\oplus k} + N_L,$$

we arrive at the Hamiltonian employed, for example, by Gamble et al. in [22].

3.2.1 Subspaces: Bosons and Fermions

For a k-particle walk, we can choose to use particles that are *indistinguishable*. These fall into two broad categories: *Bosons* and *Fermions*. Bosons are governed by Bose-Einstein statistics and are associated with symmetric states. Given a k-tuple of vertices $(x_1, ..., x_k)$ representing the locations of k particles, we associate a Boson state

$$(x_1, ..., x_k)_B = \frac{1}{\sqrt{N}} \sum_{\sigma \in S_k} (x_{\sigma(1)}, ..., x_{\sigma(k)})$$

where

$$N = \frac{k!}{\prod\limits_{j \in \Pi(\mathbf{x})} j!}$$

and S_k is the symmetric group on k elements. Note that swapping the location of any two particles leaves the state unchanged. A special case occurs when we forbid any two particles from occupying the same site. Such particles are referred to as *hard-core Bosons*.

On the other hand, Fermions obey Fermi-Dirac statistics, and are associated with anti-symmetric states. The Fermion state corresponding to $(x_1, ..., x_k)$ is

$$(x_1, ..., x_k)_F = \frac{1}{\sqrt{k!}} \sum_{\sigma \in S_k} \text{sgn}(\sigma)(x_{\sigma(1)}, ..., x_{\sigma(k)})$$

where $\text{sgn}(\sigma)$ is the sign of the permutation σ. In this case, swapping the position of any two particles induces a phase of -1. As a consequence, no two particles can be in the same location. This is known as the *Pauli exclusion principle.*

We would like to apply the multi-particle walk operators developed above to Boson and Fermion states. For this to make sense, we require a walk operator that preserves the anti-symmetric Fermion state space, and therefore also preserves the symmetric Boson state space. This is the case when the Hamiltonian H—and therefore the unitary walk operator $U(t)$—commutes with permutation of the k particles. When this is the case, we have

$$\begin{aligned} U(t)(x_1, ..., x_k)_B &= \big(U(t)(x_1, ..., x_k)\big)_B \\ U(t)(x_1, ..., x_k)_F &= \big(U(t)(x_1, ..., x_k)\big)_F \end{aligned}$$

and both the symmetric and anti-symmetric subspaces are preserved. This is the case for the generic k-particle Hamiltonians defined in the introduction of Section 3.2. In particular, this is the case for the Hamiltonian used by Gamble et al. in [22].

3.2.2 The k-Boson Invariant

In [22], Gamble et al. define an invariant using two-particle continuous time quantum walks. They consider both Bosons and Fermions, and find that the Bosons were strictly better at distinguishing non-isomorphic graphs. Here, we generalize this to k particles and focus on the case of Bosons. The Hamiltonian for this walk was defined in Section 3.2:

$$H = A^{\oplus k} + N_L.$$

Since each term commutes with permutation of the k particles, H takes Boson states to Boson states. Now, let $\{\mathbf{y}_1, ..., \mathbf{y}_\ell\}$ denote the set of Boson states on the graph G. The *Green's functions*

$$\mathcal{G} = \{f_{ij} : \ 1 \le i, j \le \ell\}$$

are functions of time defined by

$$f_{ij}(t) = \mathbf{y}_i^T U(t) \mathbf{y}_j.$$

In other words, this is the ij entry of $U(t)$ in the Boson state basis as a function of time. For their invariant, Gamble et al. consider the set

$$\mathcal{G}(t) = \{f_{ij}(t)\}$$

for a fixed time t, though they do not provide a method for choosing a value of t. For our purposes, this will be largely irrelevant—the analysis in Section 4 will apply to all choices of t. Note that the case of two hard-core Bosons corresponds to the *symmetric square* of the graph. The spectrum of the symmetric square was considered as a graph invariant by Audenaert, Godsil, Royle and Rudolph in [4]. Constructions for pairs of non-isomorphic graphs that are not distinguished by the spectra of their symmetric squares are given by Alzaga et al. [2] as well as Ponomarenko et al. [35].

It is important to note that, although the k-Boson invariant is based on a quantum walk, it is a classical algorithm; the entries of $U(t)$ are calculated classically and then considered as a set. For a fixed number of Bosons, this can be done in time polynomial in the number of vertices in G. Thus, if there existed a fixed k such that the k-Boson invariant distinguished all non-isomorphic graphs, then the graph isomorphism problem would be in P. In Section 4, we will show that this is not the case. For any k, we can construct a pair of non-isomorphic graphs that are not distinguished by the k-Boson invariant.

3.3 Discrete Time Quantum Walks

Given a graph $G = (V, E)$, the set of *arcs* $R(G)$ of the graph G consists of all ordered pairs (u, v) of vertices such that u and v are adjacent. Therefore, each edge uv gives rise to two arcs uv and vu. A *discrete time quantum walk* on a graph G takes place in the complex vector space with basis

$$\{e_{uv} : uv \in R(G)\}.$$

The transition matrix U has entries indexed by the arcs of G with values

$$U_{wx,uv} = \begin{cases} \frac{2}{\deg(v)} & v = w, u \neq x \\ \frac{2}{\deg(v)} - 1 & v = w, u = x \\ 0 & \text{otherwise.} \end{cases}$$

Discrete time quantum walks have been studied extensively in the literature on quantum computing. A more detailed presentation can be found in [38], [34] and [36].

3.3.1 A Discrete-Time Invariant

We will now outline the discrete time walk invariant introduced by Emms et al. in [17] and analyzed in depth by Godsil and Guo in [27]. In Section 3.3, we introduced a discrete time quantum walk operator U. We now define the *positive support* of a matrix:

$$S^+(M)_{uv} = \begin{cases} 1 & M_{uv} > 0 \\ 0 & \text{otherwise.} \end{cases}$$

The invariant of Emms et al. is the spectrum of

$$S^+(U^3).$$

Similar to the k-Boson invariant, this is a classical algorithm inspired by the discrete time quantum walk. It runs in time polynomial in the number of vertices. Emms et al. conjecture that this invariant can distinguish all non-isomorphic strongly regular graphs. In Section 4, we will provide a sufficient condition for a pair of graphs to be indistinguishable by this invariant, and a construction of such a pair of graphs on 512 vertices. These graphs are not strongly regular, so the conjecture of Emms et al. remains unresolved.

Chapter 4

Cellular Algebras

Cellular algebras were first studied by Weisfeiler and Lehman [40], and independently by Higman [30], who referred to them as *coherent configurations*. A cellular algebra is a matrix algebra over the complex numbers that is closed under Schur multiplication, conjugation and transposition. Additionally, it contains J, the all-ones matrix. As a consequence, a cellular algebra has a unique basis of 0-1 matrices, making it very useful for encoding incidence structures such as graphs and associated multi-particle walks.

In this chapter, we will introduce cellular algebras and their relationships to graphs. In Section 4.2, we define weak and strong isomorphisms of cellular algebras. In Section 4.3, we will introduce the k-extension of a cellular algebra—a construction that will allow us to accommodate multi-particle walks. A weak isomorphism that respects k-extensions is a k-isomorphism. Two graphs that are contained in k-isomorphic cellular algebras are referred to as k-equivalent. Our treatment of these topics will closely parallel that of Evdokimov, Ponomarenko and Karpinski [19, 18].

Section 4.5 details a novel application of the theory of cellular algebras to multi-particle quantum walks. This culminates in Theorem 4.5.4, which shows that, if two graphs are k-equivalent, then k-particle continuous time walks on these graphs share a number of characteristics. As a consequence, Theorem 4.5.5 states that k-equivalent graphs are not distinguished by the k-Boson invariant of Gamble et al. In Section 4.6, we will take a similar approach to discrete time quantum walks. Theorem 4.6.6 states that 2-equivalent graphs are not distinguished by the invariant of Emms et al.

Finally, in Section 4.7, we present a new construction for pairs of non-isomorphic k-equivalent graphs for all k. These graphs have diameter two and four eigenvalues.

4.1 Algebras from Graphs

Let V be a finite vertex set, and Mat_V the set of square complex matrices with rows and columns indexed by V. A *cellular algebra* W is a subalgebra of Mat_V such that

(i) W is closed under Schur multiplication.

(ii) W is closed under transposition and conjugation, and therefore under conjugate transposition.

(iii) W contains J, the all-ones matrix and the identity matrix I.

The following lemma is an immediate consequence of this definition:

4.1.1 Lemma. *If W is a cellular algebra, then*

(i) W has a unique basis of 01-matrices $\mathcal{A} = \{A_0, ..., A_d\}$ with $\sum_{A_i \in \mathcal{A}} A_i = J$.

(ii) There is a subset C of $\mathcal{A}$ such that $\sum_{A_i \in C} A_i = I$.

(iii) If $A_i \in \mathcal{A}$, then $A_i^\dagger \in \mathcal{A}$

We refer to $\mathcal{A}$ as the set of *basis relations* of the cellular algebra. Since the cellular algebra is closed under matrix multiplication, there is a set of scalars p_{ij}^k such that

$$A_i A_j = \sum_k p_{ij}^k A_k$$

for all i, j. The values p_{ij}^k are called the *intersection numbers* of the algebra. A set of vertices $U \subseteq V$ is called a *cell* of W if I_U, the identity on U, is a basis relation of W. The set of cells of W is denoted by $\mathrm{Cell}(W)$.

We say that a cellular algebra W is *generated* by a set of matrices $M_0, ..., M_\ell$, if it is the smallest cellular algebra containing $M_0, ..., M_\ell$ and we write

$$W = \langle M_0, ..., M_\ell \rangle .$$

In particular, given a graph G with adjacency matrix A, we will write $W_G = \langle A \rangle$. We say that W_G is the *cellular closure* of G. Any cellular algebra that contains A will be said to contain the graph G. If the cellular algebra containing G has only one cell, then we say that the graph G is *homogeneous*. The Weisfeiler-Lehman algorithm [40] determines the cellular closure in time polynomial in the size of the matrices. If A is contained in W, then any polynomial in A is also contained in W. In particular, W contains the quantum walk operator $U(t) = e^{itA}$ for all real values of t, a fact that will prove very useful in subsequent sections.

4.2 Weak and Strong Isomorphisms

We will define two notions of isomorphisms between cellular algebras—one of a combinatorial nature (strong), and the other of an algebraic nature (weak).

Let W and W' be cellular algebras with vertex sets V and V'. Then, a *weak isomorphism* is a bijection

$$\phi : W \to W'$$

that preserves addition, matrix multiplication, Schur multiplication and complex conjugation. A weak isomorphism also preserves the identity matrix I and the all-ones matrix J. We can think of this in terms of the intersection numbers of the algebras. Let W and W' be cellular algebras with intersection numbers $\{p_{ij}^k\}$ and $\{r_{ij}^k\}$ respectively. Then, if there is a bijection σ such that, for all i, j, k,

$$p_{ij}^k = r_{i^\sigma j^\sigma}^{k^\sigma}$$

then there is a weak isomorphism defined by

$$\phi_\sigma(A_i) = A'_{i^\sigma}.$$

The converse is also true—if W and W' are weakly isomorphic, then their intersection numbers must be the same.

A *strong isomorphism* is a bijection

$$\psi : V \to V'$$

such that, if S_ψ is the permutation matrix corresponding to ψ, then

$$\psi'(M) = S_\psi M S_\psi^T$$

is a weak isomorphism from W to W'. We can restate this definition in terms of basis relations. Let $\mathcal{A} = \{A_0, ..., A_\ell\}$ and $\mathcal{A}' = \{A'_0, ..., A'_\ell\}$ be the sets of basis relations for W and W'. Then ψ is a strong isomorphism if, for any j there exists some j' such that

$$\forall u, v \in V : \; A_j(u,v) = A_{j'}(\psi(u), \psi(v)).$$

A strong isomorphism induces a weak one, but the converse is not always true. Given a strong isomorphism ψ, we denote the corresponding weak isomorphism by $\widetilde{\psi}$. Deciding when two weakly isomorphic algebras are strongly isomorphic lies at the centre of the study of cellular algebras.

We will now outline some of the properties of weak isomorphisms that we will make use of in subsequent sections. Since a weak isomorphism ϕ preserves matrix multiplication and addition, we must have $\phi(I) = I$ and $\phi(J) = J$. Therefore, ϕ induces a bijection between the cells of W and those of W':

$$\phi' : \mathrm{Cell}(W) \to \mathrm{Cell}(W').$$

We can now state the following lemma:

4.2.1 Lemma. *Take $X \in Cell(W)$. Then $|X| = |\phi'(X)|$.*

Proof. Note that

$$I_X \circ (J\, I_X\, J) = |X| \cdot I_X$$

and similarly for W'

$$I_{\phi'(X)} \circ (J\, I_{\phi'(X)}\, J) = |\phi'(X)| \cdot I_{\phi'(X)}.$$

However, applying ϕ to each side of the first equation gives us

$$\phi(I_X) \circ (J\, \phi(I_X)\, J) = |X| \cdot \phi(I_X).$$

Since $\phi(I_X) = I_{\phi'(X)}$, we have $|X| = |\phi'(X)|$, as required. □

In addition to preserving the sizes of the cells, a weak isomorphism ϕ preserves several other important properties of elements of W.

4.2.2 Lemma. *Let ϕ be a weak isomorphism from W to W'. Take any $M \in W$. Then*

(i) $\mathrm{tr}(M) = \mathrm{tr}(\phi(M))$.

(ii) *M and $\phi(M)$ are cospectral.*

(iii) The matrix entries of M, taken as a list, are the same as the entries of $\phi(M)$.

Proof. Statement (i) is a direct consequence of Lemma 4.2.1. The following proof of (ii) appears in [35]. For any polynomial $p(\cdot)$, we have $\phi(p(M)) = p(\phi(M))$. In particular, M and $\phi(M)$ must have the same minimal polynomial, and thus the same eigenvalues. We now need to show that the multiplicities of the eigenvalues are the same. By (i), we know that $\mathrm{tr}(M^r) = \mathrm{tr}((\phi(M))^r)$ for any non-negative integer r. That is,

$$\forall r : \sum_i (m_i - m_i')\lambda_i^r = 0$$

where the λ_i are the shared eigenvalues of M and M' and m_i and m_i' are the respective multiplicities. If there are s distinct eigenvalues, then letting $r = 0, ..., (s-1)$ gives s linear equations. These equations define a Vandermonde matrix R whose determinant is given by

$$\det(R) = \prod_{i<j}(\lambda_i - \lambda_j)$$

which is non-zero since the eigenvalues are distinct. The only solution, therefore, is that $m_i = m_i'$ for all i. Hence M and $\phi(M)$ are cospectral.

To prove (iii), we write M as a sum of basis relations

$$M = \sum_i a_i A_i.$$

Since the basis relations are orthogonal Schur idempotents, the matrix entries of M are the values a_i. Each a_i is repeated with multiplicity m_i, the number of ones in the matrix A_i. Expressing $\phi(M)$ as

$$\phi(M) = \sum_i a_i \phi(A_i)$$

we see that the values of the matrix entries of $\phi(M)$ are the same. We need now only show that the multiplicities m_i are the same—that is, that the number of ones in A_i is the same as the number of ones in $\phi(A_i)$. The number of ones in A_i is given by $\mathrm{tr}(A_i A_i^T)$. Applying (i), we see that

$$\mathrm{tr}(A_i A_i^T) = \mathrm{tr}(\phi(A_i)\phi(A_i)^T).$$

Therefore, the multiplicities m_i are the same, and the entries of the matrices M and $\phi(M)$, when taken as a list, are identical. □

We have seen how cellular algebras can be constructed from graphs, and how these algebras may be interrelated by weak and strong isomorphisms. We will now develop a way to extend these algebras, incorporating more structural information about a graph.

4.3 Extensions of Cellular Algebras

The k-extension of a cellular algebra was defined by Ponomarenko and Evdokimov in [19], and by Barghi in [35]. The lemmas presented below are minor adaptations of those found in their work. The k-extension of an algebra W is denoted by $\widehat{W}^{(k)}$. The extension consists of matrices indexed by V^k. It contains the k-fold tensor power of W. However, the tensor product alone adds no new structure; if two cellular algebras are weakly isomorphic, then so are their k-fold tensor powers. We will therefore include some additional elements in $\widehat{W}^{(k)}$. From a physical point of view, these additional elements will allow us to describe interaction among particles, as we will see in Section 4.5. We define Δ_I, a matrix with entries indexed by elements of V^k, such that

$$(\Delta_I)_{\mathbf{x},\mathbf{y}} = \begin{cases} 1 & \text{if } \mathbf{x} = \mathbf{y} = (u, u, ..., u) \text{ for some } u \in V \\ 0 & \text{otherwise.} \end{cases}$$

This is the identity relation on the diagonal elements of V^k. We can now define the k-extension

$$\widehat{W}^{(k)} = \left\langle W^{\otimes k}, \Delta_I \right\rangle.$$

The inclusion of the element Δ_I often makes $\widehat{W}^{(k)}$ substantially larger than $W^{\otimes k}$.

We now define the *cylindric relations*, a useful subset of the k-extension. Let S be a set of 01-matrices $M_{i,j}$ of W indexed by i, j where $1 \leq i, j \leq k$:

$$S = \{M_{i,j} : \ 1 \leq i, j \leq k\}.$$

Then, the cylindric relation corresponding to S is a 01-matrix $\mathcal{C}_S$ indexed by V^k such that, for any $x, y \in V^k$,

$$(\mathcal{C}_S)_{x,y} = \begin{cases} 1 & \text{if } (M_{i,j})_{x_i,y_j} = 1 \text{ for all } i, j \\ 0 & \text{otherwise} \end{cases}$$

In other words, $\mathcal{C}_S$ relates k-tuples x and y if the i^{th} entry of x is related to the j^{th} entry of y for all i, j. We can now state the following lemma, proven by Evdokimov and Ponomarenko in [19]:

4.3.1 Lemma. *For all cylindric relations $\mathcal{C}_S$, we have $\mathcal{C}_S \in \widehat{W}^{(k)}$.*

Proof. Take any 01-matrix M in W. Define a 01-matrix $M^{(i,j)}$ such that, for any $x, y \in V^k$,

$$M^{(i,j)}_{x,y} = M_{x_i,y_j}.$$

That is, the x, y entry of $M^{(i,j)}$ is 1 if and only if x_i is related to y_j by M. Note that we can construct $M^{(i,i)}$ as follows:

$$M^{(i,i)} = \overbrace{J \otimes ... \otimes J}^{i-1} \otimes M \otimes \overbrace{J \otimes ... \otimes J}^{k-i}.$$

Then, we can write $M^{(i,j)}$ as a product:

$$M^{(i,j)} = I^{(i,i)} \Delta_I M^{(j,j)}.$$

Now, given a set $S = \{M_{i,j}\}$, we know that $M^{(i,j)}_{i,j} \in \widehat{W}^{(k)}$ for all i, j. The cylindric relation $\mathcal{C}_S$ is given by the Schur product of the $M^{(i,j)}_{i,j}$ for all i, j:

$$\mathcal{C}_S = M^{(1,1)}_{1,1} \circ M^{(1,2)}_{1,2} \circ ... \circ M^{(k,k-1)}_{k,k-1} \circ M^{(k,k)}_{k,k}.$$

Since $\widehat{W}^{(k)}$ is closed under Schur multiplication, we have $\mathcal{C}_S \in \widehat{W}^{(k)}$. □

This lemma gives us a useful set of relations in $\widehat{W}^{(k)}$. We will now see that it also identifies some of the cells of $\widehat{W}^{(k)}$. Take a set of basis relations $T = \{A_{i,j} \in \mathcal{A} : 1 \leq i < j \leq k\}$. We say that an element x of V^k is of type T if

$$\forall A_{i,j} \in T : A_{i,j}(x_i, x_j) = 1$$

The following is an easy corollary of Lemma 4.3.1:

4.3.2 Corollary. *Let Δ_T be the identity relation on all elements of V^k of type T. Then $\Delta_T \in \widehat{W}^{(k)}$.*

In particular, we see that each cell of $\widehat{W}^{(k)}$ consists of elements a single type.

4.4 k-Equivalence

In this section, we bring together all of the main ideas of this chapter—the containment of a graph within a cellular algebra, the k-extension of such an algebra, and weak isomorphisms between these extensions.

Let G and G' be graphs with adjacency matrices A and A'. Let W and W' be cellular algebras that contain G and G' respectively. Then, we say that G and G' are *equivalent* if there is a weak isomorphism $\phi : W \to W'$ such that $\phi(A) = A'$. If G and G' are equivalent, then

$$\phi(J - A - I) = J - A' - I$$

so the complements are also equivalent. The following lemma, proven in [35], demonstrates that equivalence is quite a strong relationship.

4.4.1 Lemma. *If G and G' are equivalent, then they are cospectral with cospectral complements.*

Proof. The graphs G and G' are cospectral by Lemma 4.2.2. Since they are equivalent, their complements must be equivalent, and therefore also cospectral. □

We can now generalize this definition to k-extensions. Let G and G' be graphs with adjacency matrices A and A' and a weak isomorphism ϕ such that $\phi(A) = A'$. We say that G and G' are *k-equivalent* if there is a weak isomorphism

$$\widehat{\phi} : \widehat{W}^{(k)} \to \widehat{W'}^{(k)}$$

such that

$$\widehat{\phi} \mid_{W_G^k} = \phi^k \qquad \widehat{\phi}(\Delta_I) = \Delta_I.$$

In this case, we call ϕ a *k-isomorphism*, and we say that $\widehat{\phi}$ *extends* ϕ. The following lemma, adapted from [35], tells us that a k-isomorphism behaves in a convenient way on the cylindric relations:

4.4.2 Lemma. *Let C_S be a cylindric relation on $\widehat{W}^{(k)}$. Then, if $\widehat{\phi}$ is the extension of a k-isomorphism ϕ, then*

$$\widehat{\phi}(C_S) = C_{\phi(S)}$$

where $\phi(S) = \{\phi(A) : A \in S\}$.

Proof. In Lemma 4.3.1, we showed that the cylindric relations can be constructed as products of elements of S, along with J and the identity I. Applying ϕ to each term in this product, and using the fact that $\phi(I) = I$ and $\phi(J) = J$, we conclude that $\widehat{\phi}(C_S) = C_{\phi(S)}$. □

Let σ be a permutation on k elements. Then P_σ denotes a 01-matrix whose entries are indexed by V^k such that

$$(P_\sigma)_{x,y} = \begin{cases} 1 & \text{if } x_i = y_{\sigma(i)} \text{ for all } i \\ 0 & \text{otherwise} \end{cases}$$

In other words, it has (x, y) entry of 1 when y is obtained from x by permuting its entries by σ. The following is an easy consequence of Lemma 4.4.2:

4.4.3 Corollary. *For any permutation σ, we have $P_\sigma \in \widehat{W}^{(k)}$. Furthermore, if ϕ is a k-isomorphism, then*

$$\widehat{\phi}(P_\sigma) = P_\sigma.$$ □

The following lemma shows that some sense of distance is preserved by a k-isomorphism, a fact that will be useful when considering multi-particle quantum walks.

4.4.4 Lemma. *Let B_d be a 01-matrix indexed by the vertices of G such that*

$$(B_d)_{uv} = \begin{cases} 1 & d(u, v) = d \\ 0 & \textit{otherwise.} \end{cases}$$

Define B'_d analogously for G'. Then, if ϕ is a k-isomorphism from G to G', then

$$\phi(B_d) = B'_d.$$

Proof. Let A denote the adjacency matrix of G and A' that of G'. Define $\mathcal{A}_d$ as the set of basis relations A_j in the cellular closure of G such that

$$A^r \circ A_j$$

is zero for $r < d$ and non-zero for $r = d$. Define $\mathcal{A}'_d$ analogously for G'. Then,

$$\sum_{A_j \in \mathcal{A}_d} A_j = B_d.$$

Furthermore, since $\phi(A) = A'$, we know that ϕ takes $\mathcal{A}_d$ to $\mathcal{A}'_d$. We conclude that $\phi(B_d) = B'_d$. □

Recall that, in Section 3.2, we defined the relation Δ_D for D a symmetric matrix of non-negative integers with zero on the diagonal. The entries of Δ_D are given by

$$(\Delta_D)_{x,y} = \begin{cases} 1 & d(x_i, y_j) = D_{ij} \text{ for all } i, j \\ 0 & \text{otherwise.} \end{cases}$$

Now, setting $M_{i,j} = B_{D_{ij}}$ and

$$S = \{M_{i,j} : 1 \leq i, j \leq k\},$$

we see that Δ_D can be expressed as a cylindric relation:

$$\Delta_D = \mathcal{C}_S.$$

By Lemma 4.4.2, if ϕ is a k-isomorphism, then

$$\widehat{\phi}(\mathcal{C}_S) = \mathcal{C}_{\phi(S)}.$$

In this case, the elements of S are distance relations B_d, so applying Lemma 4.4.4 gives the following corollary:

4.4.5 Corollary. *If ϕ is a k-isomorphism from G to G', then*

$$\widehat{\phi}(\Delta_D) = \Delta'_D. \qquad \square$$

We will now introduce another theorem due to Evdokimov and Ponomarenko, which is proven in [19]. It provides a very useful sufficient condition for k-equivalence. Let $\mathrm{Cell}_m(W)$ denote the set of all subsets of $\mathrm{Cell}(W)$ of size at most m. If $U \in \mathrm{Cell}_m(W)$, and $\phi : W \to W'$ is a weak isomorphism, then let ϕ_U denote the restriction of ϕ to U and $\phi(U)$ the image of U in $\mathrm{Cell}_m(W')$. We also let W_U denote the restriction of the cellular algebra W to the subset of cells U. We can now state the following theorem.

4.4.6 Theorem. *Let W and W' be cellular algebras with a weak isomorphism $\phi : W \to W'$. Assume that, for an integer $m \geq 3k$,*

(i) For any $U \in \mathrm{Cell}_m(W)$, there is a strong isomorphism $\psi : W_U \to W'_{\phi(U)}$ such that $\widetilde{\psi} = \phi_U$.

(ii) *Take $U_1, U_2 \in Cell_m(W)$, with corresponding strong isomorphisms $\psi_1 : W_{U_1} \to W'_{\phi(U_1)}$ and $\psi_2 : W_{U_2} \to W'_{\phi(U_2)}$. Then, there is strong isomorphism ρ such that*

$$(\psi_1^{-1})_{U^*}(\psi_2)_{U^*} = \rho_{U^*}$$

where $U^* = U_1 \cap U_2$, and the weak isomorphism induced by ρ is the identity.

Then, there is a k-isomorphism $\widehat{\phi} : \widehat{W}^{(k)} \to \widehat{W'}^{(k)}$ extending ϕ.

Proof. Take any basis relation A_i of $\widehat{W}^{(k)}$. Then, there is some $U \in \mathrm{Cell}_m(W)$ such that the row and column support of A_i are contained in the cells U^k. By (i), there is a strong isomorphism

$$\psi : W_U \to W'_{\phi(U)}.$$

Then, for the k-fold cartesian power, we get a strong isomorphism

$$\psi^k : W_{U^k} \to W'_{\phi(U^k)}$$

and therefore an induced weak isomorphism $\widetilde{\psi^k}$. So, we set $\widehat{\phi}(A_i) = \widetilde{\psi^k}(A_i)$. Now, assume that the support of A_i lies in $U_1 \cap U_2$. We would like to show that it doesn't matter whether we choose $U = U_1$ or $U = U_2$. By (i), U_1 and U_2 have corresponding strong isomorphisms ψ_1 and ψ_2. By (ii), we have

$$(\psi_1^k)_U^{-1}(\psi_2^k)_U = \rho_U^k.$$

In particular, ψ_1^k and ψ_2^k induce the same weak isomorphism:

$$\widehat{\phi} = \widetilde{\psi_1^k} = \widetilde{\psi_2^k}.$$

Therefore, the choice of $U = U_1$ or $U = U_2$ does not change $\widehat{\phi}(A_i)$.

Take any two basis relations A_i, A_j. Then, if $A_iA_j \neq 0$, then the union of the row and colums support for A_i and A_j must lie in U^k for some $U \in \mathrm{Cell}_m(W)$, since $m \geq 3k$. By (i), there is a strong isomorphism $\psi : W_U \to W'_{\phi(U)}$. As discussed above, we have

$$\widehat{\phi}(A_iA_j) = \widetilde{\psi^k}(A_iA_j) = \widetilde{\psi^k}(A_i)\widetilde{\psi^k}(A_j).$$

The same holds for Schur multiplication. Thus, $\widehat{\phi}$ is a k-isomorphism from $\widehat{W}^{(k)}$ to $\widehat{W'}^{(k)}$ extending ϕ. □

4.5 k-Equivalence and Continuous Time Quantum Walks

We will show that, if G and G' are k-equivalent, then k-particle walks on these graphs will share several properties. In particular, we will see that the k-Boson invariant of Gamble et al. [22] is unable to distinguish such a pair of graphs. Recall that, in Section 3.2, we set two restrictions on the quantum walks we consider:

(i) Movement of the particles should be governed by the structure of the graph.

(ii) Interactions between a set of particles is based only on their pairwise distances in the graph.

The Hamiltonian for a k-particle walk on a graph G consists of a *movement term* M and an *interaction term* N:

$$H = M + N.$$

We consider a very general movement term

$$M = \sum_i a_i M_i$$

where M_i is a tensor product of copies of A and I.

In Section 3.2, we defined a relation Δ_D such that

$$(\Delta_D)_{\mathbf{x},\mathbf{y}} = \begin{cases} 1 & d(x_i, y_j) = D_{ij} \text{ for all } i, j \\ 0 & \text{otherwise} \end{cases}$$

for D a $k \times k$ matrix. We then wrote our interaction term as

$$N = -\sum_j b_j \Delta_{D_j}$$

for $n \times n$ matrices D_j with non-negative entries and zero on the diagonal. We can now state the following lemma:

4.5.1 Lemma. *For a graph G with cellular closure W, any k-particle Hamiltonian $H = M + N$ as described above is contained in the k-extension $\widehat{W}^{(k)}$.*

Proof. We write

$$H = M + N = \sum_i a_i M_i - \sum_j b_j \Delta_{D_j}.$$

By the definition of the k-extension, $M_i \in \widehat{W}^{(k)}$. By Lemma 4.4.4, we also have $\Delta_{D_j} \in \widehat{W}^{(k)}$. Since H is a linear combination of these elements, $H \in \widehat{W}^{(k)}$. □

While the Hamiltonian H applies to the graph G, we denote by $H' = M' + N'$ the identical Hamiltonian acting on G'.

4.5.2 Theorem. *Let G and G' be k-equivalent graphs, with Hamiltonians for some k-particle walk H and H'. Then,*

$$\widehat{\phi}(H) = H'.$$

Proof. First consider the movement terms M and M'. We know that $M_i \in W^{\otimes k}$ and $M_i' \in (W')^{\otimes k}$, and therefore,

$$\widehat{\phi}(M_i) = \phi^k(M_i).$$

Since ϕ is a weak isomorphism with $\phi(I) = I$ and $\phi(A) = A'$, we have $\widehat{\phi}(M_i) = M_i'$. Corollary 4.4.5 gives us

$$\widehat{\phi}(\Delta_{D_j}) = \Delta'_{D_j}$$

for all j. Therefore $\widehat{\phi}(N) = N'$ and $\widehat{\phi}(H) = H'$. □

4.5.3 Corollary. *For any time t,*

$$\widehat{\phi}(e^{-itH}) = e^{-itH'}.$$

Proof. Since e^{-itH} is a polynomial in H and $\widehat{\phi}(H) = H'$, we have $\widehat{\phi}(e^{-itH}) = e^{-itH'}$. □

This result suggests that k-particle walks on two k-equivalent graphs should share many properties. The following lemma identifies some of these similarities.

4.5.4 Theorem. *Let G and G' be a pair of k-equivalent graphs. Let H and H' be the Hamiltonians for a k-particle quantum walk on G and G'. Then,* *(i)* $\mathrm{tr}(H) = \mathrm{tr}(H')$ *and* $\mathrm{tr}(e^{-itH}) = \mathrm{tr}(e^{-itH'})$ *for all* t.

(ii) H *and* H' *are cospectral, as are* e^{-itH} *and* $e^{-itH'}$ *for all* t.

(iii) The entries of H*, when taken as a list, are the same as those of* H'.

(iv) Let $f_{ij}(t)$ *(resp.* $f'_{ij}(t)$*) be the* ij *entry of* e^{-itH} *(resp.* $e^{-itH'}$*) as a function of time* t*. Let* $F = \{f_{ij}\}$ *and* $F' = \{f'_{ij}\}$*. Then,* $F = F'$.

Proof. These are direct consequences of Theorem 4.5.2 and Lemma 4.2.2. □

This theorem gives us a family of properties (i)-(iv) that are shared by pairs of k-equivalent graphs. Any graph invariant derived from these properties will fail to distinguish k-equivalent graphs. The k-Boson invariant of Gamble et al. [22] does not quite fall into this category, since it considers a basis of Boson states. However, in the next section, we will see how Theorem 4.5.4 can be adapted slightly and applied to the k-Boson invariant as well.

4.5.1 The k-Boson Invariant

A *partition* Π of the positive integer k is a set of non-negative integers that sum to k. Given a k-particle state $\mathbf{x}$, let $v(\mathbf{x})$ denote the number of particles at vertex $\mathbf{x}$. Then, the partition induced by $\mathbf{x}$ is

$$\Pi(\mathbf{x}) = \{v(\mathbf{x}) : v \in V\}.$$

Given a partition Π of k, we define the operator Δ_Π as follows:

$$(\Delta_\Pi)_{\mathbf{x},\mathbf{y}} = \begin{cases} 1 & \mathbf{x} = \mathbf{y} \text{ and } \Pi(\mathbf{x}) = \Pi \\ 0 & \text{otherwise.} \end{cases}$$

That is, it acts as the identity on states $\mathbf{x}$ that induce the partition Π. Note that Δ_Π can easily be constructed as a cylindric relation, so it is contained in the k-extension and is preserved by k-isomorphism. Recall that the operator P_σ was defined as follows:

$$(P_\sigma)_{\mathbf{x},\mathbf{y}} = \begin{cases} 1 & \text{if } \mathbf{x}_i = \mathbf{y}_{\sigma(i)} \text{ for all } i \\ 0 & \text{otherwise} \end{cases}$$

and that, for any $\mathbf{x} \in V^k$, the Boson state associated with $\mathbf{x}$ is

$$\mathbf{x}_B = \frac{1}{\sqrt{N}} \sum_{\sigma \in S_k} P_\sigma \mathbf{x}$$

for

$$N = \frac{k!}{\prod_{j \in \Pi(\mathbf{x})} j!}\,.$$

So, we can define an operator B_Π that takes states $\mathbf{x}$ that induce the partition Π to their Boson states:

$$B_\Pi = \frac{1}{\sqrt{N}} \sum_{\sigma \in S_k} P_\sigma \Delta_\Pi.$$

Now, take a k-particle walk Hamiltonian H that commutes with P_σ for all σ. Then, the associated unitary $U(t)$ takes Boson states to Boson states. Now, define the operator

$$U_\Pi(t) = B_\Pi^T U(t) B_\Pi.$$

Then, for $\mathbf{x} \in V^k$, we have

$$\mathbf{x}^T U_\Pi(t)\mathbf{y} = \begin{cases} \mathbf{x}_B^T U(t)\mathbf{y}_B & \Pi(\mathbf{x}) = \Pi(\mathbf{y}) = \Pi \\ 0 & \text{otherwise.} \end{cases}$$

That is, it gives the Green's function associated with the Boson states $\mathbf{x}_B$ and $\mathbf{y}_B$. However, we note that there are

$$N = \frac{k!}{\prod_{j \in \Pi(\mathbf{x})} j!}$$

k-particle basis states $\mathbf{x}$ that give the same Boson state. Therefore, considering the set

$$\mathcal{G}_\Pi(t)' = \{\mathbf{x}^T U_\Pi(t)\mathbf{y} : \mathbf{x}, \mathbf{y} \in V^k\}$$

we find each value counted N^2 times. Removing this repetition gives us the desired set of Green's functions $\mathcal{G}_\Pi(t)$. Taking the union

$$\mathcal{G}(t) = \bigcup_\Pi \mathcal{G}_\Pi(t)$$

gives us the desired Green's functions. We know that, if G and G' are k-equivalent with k-isomorphism ϕ, then

$$\widehat{\phi}(U(t)) = U'(t)$$

and that $\widehat{\phi}$ preserves B_Π for all Π. Therefore, for each Π,

$$\mathcal{G}_\Pi(t) = \mathcal{G}'_\Pi(t)$$

and therefore

$$\mathcal{G}(t) = \mathcal{G}'(t).$$

This gives us the following theorem:

4.5.5 Theorem. *If G and G' are k-equivalent graphs, then they are not distinguished by any k-Boson invariant.* □

4.6 k-Equivalence and Discrete Time Quantum Walks

The digraph $D = D(G)$ is constructed from G by replacing each edge with a pair of arcs directed in opposite directions. The discrete time quantum walk takes place on the arcs of D. Its evolution is governed by the unitary matrix $U = U(G)$, which is defined by

$$U_{wx,uv} = \begin{cases} \frac{2}{\deg(v)} & v = w \text{ and } u \neq x \\ \frac{2}{\deg(v)} - 1 & v = w \text{ and } u = x \\ 0 & \text{otherwise.} \end{cases}$$

We can write this in a more compact form as follows:

$$U_{wx,uv} = \delta_{vw}\left(\frac{2}{\deg(v)} - \delta_{ux}\right). \tag{4.6.1}$$

Emms et al. [17] define a graph invariant by taking the positive support of the cube of the walk operator: $S^+(U^3)$ and considering its spectrum. Here, the positive support is defined by

$$S^+(M)_{ij} = \begin{cases} 1 & M_{ij} > 0 \\ 0 & \text{otherwise.} \end{cases}$$

Guo and Godsil [27] also explore this invariant, showing that the spectra of $S^+(U)$ and $S^+(U^2)$ are determined by the spectrum of G, and are thus insufficient for distinguishing cospectral graphs. In this section, we will show that, for any k, the set $\mathrm{spec}(S^+(U^k))$ is the same for any pair of 2-equivalent graphs, and therefore such pairs of graphs are indistinguishable by this invariant. We begin with the following lemma:

4.6.1 Lemma. *Let V_r be the set of vertices of G of degree r, and I_r be the identity relation on V_r. Then, I_r is contained in W, the cellular closure of G.*

Proof. Consider the diagonal of A^2:

$$I \circ A^2 = \sum_r r I_r.$$

Thus, each I_r must be a sum of basis relations of W, and is therefore contained in W. □

We will now show that U, U^k and $S^+(U^k)$ are contained in the two extension $\widehat{W}^{(2)}$. Furthermore, we will show that a 2-equivalence preserves these elements, ensuring that they are cospectral for 2-equivalent graphs .

4.6.2 Lemma. *The walk operator U is contained in the 2-extension $\widehat{W}^{(2)}$ of G.*

Proof. Since $I_r \in W$, the set $\{(v, v) : \deg(v) = r\}$ is a union of cells in $\widehat{W}^{(2)}$. Therefore, the identity relation on this union of cells is in $\widehat{W}^{(2)}$. Denote this relation by Δ_{I_r}. The matrix

$$(A \otimes I)\Delta_{I_r}(A \otimes I)$$

has a 1 in entry (xw, uv) if and only if $w = v$ and $\deg(v) = r$. To get the proper weights on the diagonal and off-diagonal entries, we can take the Schur product with

$$\frac{2}{r}J - I.$$

These weights come directly from Equation 4.6.1. Now, let τ be the "swap" permutation of two elements, and let A_τ be the corresponding relation on V^2. Then, A_τ is a cylindric relation, so by Lemma 4.3.1, $A_\tau \in \widehat{W}^{(2)}$. We can now use these matrices to construct U as follows:

$$U = A_\tau \left(\sum_k \left(\frac{2}{k} J + I \right) \circ \Big((A \otimes I)\Delta_{I_k}(A \otimes I) \Big) \right).$$

Since U is obtained from elements of $\widehat{W}^{(2)}$ by matrix multiplication, Schur multiplication and addition, U is contained in $\widehat{W}^{(k)}$. □

Next, we will show that a 2-equivalence respects the walk operator U:

4.6.3 Theorem. *Let G and G' be 2-equivalent graphs with walk operators U and U'. If ϕ is the 2-isomorphism relating G and G', then $\widehat{\phi}(U) = U'$.*

Proof. We know that $\widehat{\phi}(J) = J$, $\widehat{\phi}(I) = I$ and $\widehat{\phi}(A \otimes I) = A' \otimes I$. Furthermore, $\phi(A_\tau) = A_\tau$ by Lemma 4.4.2. Thus, we need only show that $\phi(\Delta_{I_k}) = \Delta_{I'_k}$. Consider the product $\Delta_I(A \otimes I)^2 \Delta_I$. For any non-zero k, the entries of $\Delta_I(A \otimes I)^2 \Delta_I$ with value k are (vv, vv) where v is a vertex of G with degree k. That is, the sub matrix of $\Delta_I(A \otimes I)^2 \Delta_I$ with value k is exactly kI_k. Now,

$$\widehat{\phi}(\Delta_I(A \otimes I)^2 \Delta_I) = \Delta_I(A' \otimes I)^2 \Delta_I.$$

Since $\widehat{\phi}$ is linear and takes the basis relations of W to the basis relations of W', it must map the submatrix of $\Delta_I(A \otimes I)^2 \Delta_I$ with entries equal to k to the submatrix of $\Delta_I(A' \otimes I)^2 \Delta_I$ with entries equal to k. Equivalently, $\widehat{\phi}(I_k) = I'_k$. Therefore, $\widehat{\phi}(U) = U'$. □

4.6.4 Corollary. *For all $k \in \mathbb{Z}^+$, we have $\widehat{\phi}(U^k) = (U')^k$.*

4.6.5 Corollary. *For all $k \in \mathbb{Z}^+$, we have $\widehat{\phi}(S^+(U^k)) = S^+((U')^k)$.*

Proof. We can write U^k as a sum of basis relations of $\widehat{W}^{(2)}$. Let $\mathcal{S}^+(U^k)$ be the set of basis relations that have positive weight in this sum. Similarly, let $\mathcal{S}^+((U')^k)$ denote the set of basis relations of $\widehat{W'}^{(2)}$ that have positive weight on $(U')^k$. Then, since $\widehat{\phi}$ maps basis relations to basis relations, and is linear, it must take $\mathcal{S}^+(U^k)$ to $\mathcal{S}^+((U')^k)$. Now, we can write

$$\widehat{\phi}(S^+(U)) = \sum_{A_i \in \mathcal{S}^+(U^k)} \widehat{\phi}(A_i) = \sum_{A_j \in \mathcal{S}^+((U')^k)} A_j = S^+((U')^k).$$ □

We can now state the following theorem, which is analogous to Theorem 4.5.4.

4.6.6 Theorem. *Let G and G' be a pair of k-equivalent graphs. Let U and U' be the discrete time walk operators defined by 4.6.1. Then, for any $k \in \mathbb{Z}^+$*

(i) $\operatorname{tr}(U^k) = \operatorname{tr}((U')^k)$ *and* $\operatorname{tr}(S^+(U^k)) = \operatorname{tr}(S^+((U')^k))$.

(ii) U^k *and* $(U')^k$ *are cospectral, as are* $S^+(U^k)$ *and* $S^+((U')^k)$.

(iii) The entries of U^k and $(U')^k$, when taken as a list, are identical. The same applies to $S^+(U^k)$ and $S^+((U')^k)$.

Proof. These are direct consequences of the definition of Theorem 4.6.3, along with its corollaries, as well as Lemma 4.2.2. □

In particular, this theorem tells us that the discrete walk invariant proposed by Emms et al. in [17] cannot distinguish a pair of 2-equivalent graphs.

4.7 Constructions

We begin with a connected graph H with minimum degree at least two. We will construct the graph $G = G(H)$ by replacing each vertex u of H with a set of vertices V_u. We will refer to these sets V_u a the *cells* of the graph G. The sizes of the cells, as well as the connections between them will be determined by the structure of H.

Let u be a vertex of H. Let E_u denote the set of edges incident at u. Then, the vertices of V_u are the subsets of E_u of even size. We will denote each subset by a 01-vector indexed by E_u. That is,

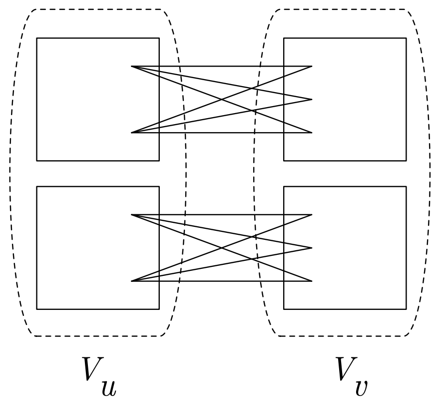
$$V_u = \{(u, \mathbf{x}) \,:\, \mathbf{x} \in \mathbb{Z}_2^{E_u},\ |\mathbf{x}| \text{ even}\}$$

where $|\mathbf{x}|$ denotes the Hamming weight of $\mathbf{x}$.

The vertices of each cell will form a co-clique in G. We will now describe how the vertices of two cells are connected. Let u and v be vertices in H with corresponding cells V_u and V_v in G. If u and v are not adjacent in H, then there are no edges between V_u and V_v in G. If u and v are adjacent in H, then let $e = (u, v)$ be the edge that connects them. Now, take $(u, \mathbf{x}) \in V_u$ and $(v, \mathbf{y}) \in V_v$. Then, $(u, \mathbf{x})$ and $(v, \mathbf{y})$ are adjacent in G if $\mathbf{x}_e = \mathbf{y}_e$. In other words, each edge incident at u partitions the vertices of V_u into two halves—those with $\mathbf{x}_e = 0$ and those with $\mathbf{x}_e = 1$. The vertices of V_v are partitioned similarly. The corresponding halves are then completely connected. This is illustrated in Figure 4.7.1.

We will now define a *twisting* operation $\mathcal{T}_{uv}$, which we will apply to G to obtain a graph $\mathcal{T}_{uv}(G)$. Let u and v be adjacent vertices in H. Then, the operation $\mathcal{T}_{uv}$ consists of removing all of the edges between V_u and V_v and replacing them with all of the non-edges between V_u and V_v. That is, if $(u, \mathbf{x}) \in V_u$ and $(v, \mathbf{y}) \in V_v$, then $(u, \mathbf{x})$ and $(v, \mathbf{y})$ are adjacent in $\mathcal{T}_{uv}(G)$ if and only if they are not adjacent in G. We will say that we are applying

Figure 4.7.1: The connections between two cells.



a twist at location uv. We will now prove several important properties of G and $\mathcal{T}_{uv}(G)$.

4.7.1 Lemma. *Let u, v, w be vertices of H such that $uv \in E(H)$ and $vw \in E(H)$. Then,*

$$\mathcal{T}_{uv}(\mathcal{T}_{vw}(G)) \cong G.$$

Proof. Let $e_1 = (u, v)$ and $e_2 = (v, w)$. Let $\mathbf{z} \in \mathbb{Z}_2^{E_v}$ be a vector with $\mathbf{z}_{e_1} = 1$, $\mathbf{z}_{e_2} = 1$, and zeroes in all other entries. Then, it is easily verified that the mapping

$$\psi_{uvw} : (v, \mathbf{x}) \to (v, \mathbf{x} + \mathbf{z})$$

is an isomorphism from $\mathcal{T}_{uv}(\mathcal{T}_{vw}(G))$ to G. □

4.7.2 Corollary. *For u and w neighbours of v,*

$$\mathcal{T}_{uv}(G) \cong \mathcal{T}_{vw}(G).$$

Proof. Each twisting operation $\mathcal{T}_{uv}$ is its own inverse. Therefore, Lemma 4.7.1 tells us that $\mathcal{T}_{uv}(G) \cong \mathcal{T}_{vw}(G)$. □

4.7.3 Corollary. *For any edges uv and xy in H,*

$$\mathcal{T}_{uv}(G) \cong \mathcal{T}_{xy}(G).$$

Proof. Since H is connected, there is a path connecting uv and xy. Repeated applications of Lemma 4.7.2 gives us $\mathcal{T}_{uv}(G) \cong \mathcal{T}_{xy}(G)$. □

We can interpret this corollary as follows: beginning with the graph G, if we apply an even number of twists, we arrive at a graph isomorphic to G; if we apply an odd number of twists, we arrive at a graph isomorphic to $\mathcal{T}_{uv}(G)$ for uv an edge in H. Note that these two isomorphism classes may be the same, depending on the underlying graph H.

We will now identify a cellular algebra $W = W(H)$ that contains both G and $\mathcal{T}_{uv}(G)$. It should be pointed out that this algebra will not, in general, be the smallest one containing G, nor the smallest containing $\mathcal{T}_{uv}(G)$. Rather, it is chosen because it will allow us to apply Theorem 4.4.6 to show k-equivalence of G and $\mathcal{T}_{uv}(G)$ for properly chosen H. The cells of this algebra will be the cells V_u for $u \in V(H)$. We will first describe the basis relations within each cell; we will then describe the relations between the cells.

Recall that the vertices of the cell V_u are of the form $(u, \mathbf{x})$. For each vector $\mathbf{z}$ in U, we now define a basis relation $C^u_{\mathbf{z}}$ as follows:

$$(C^u_z)_{(u,\mathbf{x}),(u,\mathbf{y})} = \begin{cases} 1 & \text{if } \mathbf{x} + \mathbf{z} = \mathbf{y} \\ 0 & \text{otherwise.} \end{cases}$$

That is, it relates $(u, \mathbf{x})$ and $(u, \mathbf{y})$ if $\mathbf{x} + \mathbf{z} = \mathbf{y}$. Note that $C^u_{\mathbf{z}}$ is symmetric, and that C^u_0 is the identity relation on the cell V_u.

We will now describe the two basis relations from a cell V_u to a cell V_v. These two relations will be denoted by A^{uv} and B^{uv}. A^{uv} is the adjacency matrix of G restricted to the rows indexed by V_u and the columns indexed by V_v. B^{uv} is the complement of the adjacency matrix of G restricted in the same way. More formally, the entries indexed by vertices $(u, \mathbf{x})$ and $(v, \mathbf{y})$ are defined as follows:

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

$$B^{uv}_{(u,\mathbf{x}),(v,\mathbf{y})} = \begin{cases} 1 & \text{if } ((u, \mathbf{x}), (v, \mathbf{y})) \notin E(G) \\ 0 & \text{otherwise.} \end{cases}$$

Both matrices are zero on all entries not indexed by a vertex of V_u and a vertex of V_v. Note that, if $uv \notin E(H)$, then A^{uv} is the all-zeros matrix, and need not be considered a basis relation of our algebra; it is included above for the sake of a compact definition. Neither of these matrices is symmetric, but

$$(A^{uv})^T = A^{vu} \qquad (B^{uv})^T = B^{vu}.$$

We now assemble these relations in a single set $\mathcal{A}$:

$$\begin{aligned}\mathcal{A} =&\{A^{uv} \,:\, uv \in E(H)\}\\ &\cup \{B^{uv} \,:\, u, v \in V(H), u \neq v\}\\ &\cup \{C_z^u \,:\, u \in V(H), \mathbf{z} \in \mathbb{Z}_e^{E_u},\ |\mathbf{z}| \text{ even}\}\end{aligned}$$

and make the following claim:

4.7.4 Lemma. *$\mathcal{A}$ is a set of basis relations of a cellular algebra.*

Proof. We first verify that I and J are contained in the span of $\mathcal{A}$:

$$J = \sum_{X \in \mathcal{A}} X \qquad I = \sum_{u \in V(H)} C_0^u.$$

We have already verified that $\mathcal{A}$ is closed under transposition. Since $\mathcal{A}$ contains only 01-matrices, their span is also closed under conjugation. All of the matrices in $\mathcal{A}$ are Schur idempotent, and the Schur product of any two distinct members of $\mathcal{A}$ is zero. Therefore, their span is closed under Schur multiplication. We now need only verify that span($\mathcal{A}$) is closed under matrix multiplication. We will consider four types of matrix products:

(i) Products of two relations of type $C_{\mathbf{z}}^u$. The definition of these basis relations easily yields

$$C_{\mathbf{y}}^u C_{\mathbf{z}}^u = C_{\mathbf{z}+\mathbf{y}}^u.$$

(ii) Products between one relation of type $C_{\mathbf{z}}^u$ and another of type A^{uv} or B^{uv}. These products depend on two things—whether $uv \in E(H)$ and entry $c_u(v)$ of the vector $\mathbf{z}$. If $uv \in E(H)$ and $\mathbf{z}_{c_u(v)} = 0$, then

$$C_{\mathbf{z}}^u A^{uv} = A^{uv} \qquad C_{\mathbf{z}}^u B^{uv} = B^{uv}.$$

If $uv \in E(H)$ but $\mathbf{z}_{c_u(v)} = 1$, then

$$C_{\mathbf{z}}^u A^{uv} = B^{uv} \qquad C_{\mathbf{z}}^u B^{uv} = A^{uv}.$$

Finally, if $uv \notin E(H)$, then

$$C_{\mathbf{z}}^u A^{uv} = 0 \qquad C_{\mathbf{z}}^u B^{uv} = B^{uv}.$$

To reverse the order of the matrices in each product, we can take the transpose of both sides of these equations.

(iii) Products between a relation of the type $D^{uv}E^{uv}$ where $E^{uv} \in \{A^{uv}, B^{uv}\}$ and $D^{vw} \in \{A^{vw}, B^{vw}\}$ with $u \neq w$. In this case,

$$D^{uv}E^{vw} = \alpha\,(A^{uw} + B^{uw})$$

where α takes a value in $\{0, 2^{\deg(v)-1}, 2^{\deg(v)-2}, 2^{\deg(v)-3}\}$, depending on the choice of E^{uv}, D^{vw}, as well as whether uv and vw are edges in H.

(iv) Products of the type $A^{uv}A^{vu}$, $A^{uv}B^{vu}$, $B^{uv}A^{vu}$ or $B^{uv}B^{vu}$. If uv is an edge in H, then

$$A^{uv}A^{vu} = B^{uv}B^{vu} = 2^{\deg(v)-2} \cdot \sum_{\mathbf{z}_{c_u(v)}=0} C^u_{\mathbf{z}}$$

and

$$A^{uv}B^{vu} = B^{uv}A^{vu} = 2^{\deg(v)-2} \cdot \sum_{\mathbf{z}_{c_u(v)}=1} C^u_{\mathbf{z}}.$$

If uv is not an edge of H, then

$$A^{uv}A^{vu} = B^{uv}A^{vu} = B^{uv}A^{vu} = 0$$

and

$$B^{uv}B^{vu} = 2^{\deg(v)-1} \cdot \sum_{\mathbf{z}\in U} C^u_{\mathbf{z}}.$$

All other products are zero, and therefore, the span of $\mathcal{A}$ is closed under matrix multiplication, and $\mathcal{A}$ is a set of basis relations for a cellular algebra, W. □

Letting A and A' be the adjacency matrices of G and $\mathcal{T}_{uv}(G)$, respectively, we see that both are contained in W:

$$A = \sum_{wx\in E(H)} A^{wx} \qquad \text{and} \qquad A' = A - A^{uv} - A^{vu} + B^{uv} + B^{vu}.$$

We would now like to identify some properties of the underlying graph H that result in a k-equivalent pair of graphs G and $\mathcal{T}_{uv}(G)$. We first note that, for any edge uv of H, the matrices A^{uv} and B^{uv} are interchangeable in the products (i)-(iv) above. This gives us the following lemma:

4.7.5 Lemma. *The graphs G and $\mathcal{T}_{uv}(G)$ are 1-equivalent.; that is, there is a weak isomorphism $\phi : W \to W$ that takes G to $\mathcal{T}_{uv}(G)$. As a result, they are cospectral with cospectral complements.* □

To prove k-equivalence for larger k, we would like to apply Theorem 4.4.6. Let $\binom{V(H)}{m}$ denote the set of all subsets of $V(H)$ of size m. If $S \in \binom{V(H)}{m}$, we say that an edge is contained in S if both of its endpoints are in S. We can now state the following theorem:

4.7.6 Theorem. *Let $\binom{V(H)}{3k} = \{S_1, ..., S_\ell\}$. If, for each S_i, we can assign an edge e_i of H such that*

(a) The edge e_i is not contained in S_i

(b) For any S_i, S_j, there is a path P_{ij} in H that begins at e_i, ends at e_j and uses no edge contained in $S_i \cap S_j$.

Then, the graphs $G = G(H)$ and $\mathcal{T}_{uv}(G)$ are k-equivalent.

Proof. Given a path $P = (v_1, v_2, ..., v_r)$ in H, we define a permutation of $V(G)$:

$$\psi_P = \psi_{v_r v_{r-1} v_{r-2}} \circ ... \circ \psi_{v_4 v_3 v_2} \circ \psi_{v_3 v_2 v_1}$$

where ψ_{uvw} is as defined in Lemma 4.7.1. The permutation maps $\mathcal{T}_{v_1 v_2}(G)$ to $T_{v_{r-1} v_r}(G)$ by "moving" the twisted edge along the path P. For each path P_i, assume we have an edge e_i that satisfies (a) and (b) above. Let P_i be a path beginning on the edge uv and ending on the edge e_i. Let P_{ij} be a path beginning on the edge e_i and ending on the edge e_j, such that no edge in P_{ij} is contained in $S_i \cap S_j$. The permutations ψ_{P_i} and $\psi_{P_{ij}}$ will form the basis of this proof.

Since each vertex in H corresponds to a cell in W, each S_i has a corresponding subset of cells $U_i \in \mathrm{Cell}_{3k}(W)$. By Lemma 4.7.5, we have a weak isomorphism ϕ that takes G to $\mathcal{T}_{uv}(G)$. We will now show that we can use ϕ, along with the permutations ψ_P to satisfy requirements (i) and (ii) of Theorem 4.4.6:

(i) For any $U_i \in \mathrm{Cell}_{3k}(W)$, the restriction of ψ_{P_i} to U_i is a strong isomorphism

$$(\psi_{P_i})_{U_i} : W_{U_i} \to W_{U_i}$$

such that the weak isomorphism it induces agrees with ϕ_{U_i}:

$$\left(\widetilde{\psi_{P_i}}\right)_{U_i} = \phi_{U_i}.$$

(ii) For any U_i, U_j, let $U^* = U_i \cap U_j$. Let P_i^{-1} denote the reverse of the path P_i. Define

$$\rho = \psi_{P_i^{-1}} \psi_{P_{ji}} \psi_{P_j}.$$

Then, since $P_i^{-1} P_{ji} P_j$ is a closed walk, ρ is a strong isomorphism from W to itself, and the weak isomorphism induced by ρ is the identity. After noting that $\psi_{P_i}^{-1} = \psi_{P_i^{-1}}$, we can write

$$\left(\psi_{P_i}^{-1}\right)_{U^*} (\psi_{P_j}) = \rho_{U^*}.$$

So, if conditions (a) and (b) hold, then conditions (i) and (ii) of Theorem 4.4.6 are satisfied. In this case, G and $\mathcal{T}_{uv}(G)$ are k-equivalent. □

Ponomarenko and Evdokimov [19] give a construction that is a particular case of the one described here. A *separator* of a graph H is a subset of vertices $S \in V(H)$ such that no connected component of $H \setminus S$ contains more than $\frac{|V(H)|}{2}$ vertices. Ponomarenko and Evdokimov show that, if H is a cubic graph with no separator of size $\leq 3k$, then the graphs $G = G(H)$ and $\mathcal{T}_{uv}(G)$ are k-equivalent.

We can show that this is a consequence of Theorem 4.7.6. For each $S_i \in \binom{V(H)}{3k}$, let C_i denote the largest connected component of $H \setminus S_i$. To satisfy (a), we take any e_i in C_i. Since $|C_i| > \frac{|V(H)|}{2}$, we know that $C_i \cap C_j \neq \emptyset$ for any i, j. Therefore, we can choose a path P_{ij} from e_i to e_j which lies outside $S_i \cap S_j$. Therefore, G and $\mathcal{T}_{uv}(G)$ are k-equivalent. Although it includes the graphs of Ponomarenko and Evdokimov, the construction presented in this section is significantly more general.

4.7.1 The Case $H = K_\ell$

Emms et al. [17] conjecture that the discrete time graph invariant is able to distinguish any pair of non-isomorphic strongly regular graphs. At this point, there are no known counterexamples to this claim. The same holds for the 2-Boson invariant—it has distinguished every pair of non-isomorphic strongly regular graphs that it has been given. Therefore, finding a pair of k-equivalent strongly regular graphs would be significant. In general, the construction presented here does not yield strongly regular graphs. However, it gives graphs with diameter two and four distinct eigenvalues. This is the smallest diameter and fewest eigenvalues of any known pair of k-equivalent graphs.

We will choose our underlying graph H to be a complete graph on an even number of vertices $\ell \geq 4$. We label the vertices of K_ℓ with $0, 1, ..., (\ell - 1)$. Although the choice is arbitrary, we will apply the twisting operation at edge 01, giving the graph $\mathcal{T}(G) = \mathcal{T}_{01}(G)$. We will first prove that G (and therefore $\mathcal{T}(G)$) has exactly four eigenvalues for $\ell \geq 6$, and three eigenvalues for $\ell = 4$. Next, we will show that, for any k, we can choose ℓ so that G and $\mathcal{T}(G)$ satisfy Theorem 4.7.6, and are therefore k-equivalent. Finally, we will prove that G and $\mathcal{T}(G)$ are not isomorphic.

4.7.7 Lemma. *When $H = K_\ell$, the graph G has $\ell \cdot 2^{\ell-2}$ vertices and eigenvalues*

$$\left(2^{\ell-3}(\ell-1), -2^{\ell-3}, 2^{\ell-3}, 0\right)$$

with multiplicities

$$\left(1, \binom{\ell}{2} + \ell - 1, \binom{\ell}{2}, \ell(2^{\ell-2} - \ell)\right)$$

respectively.

Proof. We will consider five families of eigenvectors, then show that they constitute a complete set using their multiplicities.

(i) G is regular with degree $2^{\ell-3}(\ell-1)$, so the all-ones vector is an eigenvector with multiplicity one.

(ii) Let β' be an eigenvector of K_ℓ. We define a vector β indexed by the vertices of G as follows:

$$\beta_{(u,\mathbf{x})} = \beta'_u.$$

Since each vertex in V_u is adjacent to exactly $2^{\ell-3}$ vertices in each other cell, the vector β is an eigenvector with eigenvalue $-2^{\ell-3}$. Since K_ℓ has $\ell - 1$ such eigenvectors β', this results in $\ell - 1$ eigenvectors of G with eigenvalue $-2^{\ell-3}$.

(iii) Take any two cells V_u and V_v of G. Let

$$V_{uv}^j = \{(u, \mathbf{x}) \,:\, \mathbf{x}_{c_u(v)} = j\} \qquad V_{vu}^j = \{(v, \mathbf{y}) \,:\, \mathbf{y}_{c_v(u)}\}.$$

for $j = 0, 1$. In other words, all the vertices in V_{uv}^0 are connected to all the vertices in V_{vu}^0 and all the vertices in V_{uv}^1 are connected to all the vertices in V_{vu}^1. Let λ_{uv} be a vector, indexed by vertices of G, such that λ_{uv} takes the values $(-1)^j$ on V_{uv}^j, $(-1)^{j+1}$ on V_{vu}^j for $j = 0, 1$, and zero everywhere else. Then λ_{uv} is an eigenvector with eigenvalue $-2^{\ell-3}$. Since there are $\binom{\ell}{2}$ pairs of cells, there are $\binom{\ell}{2}$ such eigenvectors.

(iv) For any cells V_u and V_v, let V_{uv}^j and V_{vu}^j be defined as above. Let γ_{uv} be a vector indexed by the vertices of G such that γ_{uv} takes the values $(-1)^j$ on V_{uv}^j and V_{vu}^j for $j = 0, 1$, and zero everywhere else. Then, γ_{uv} is an eigenvector with eigenvalue $2^{\ell-3}$. There are $\binom{\ell}{2}$ pairs of cells, each yielding an eigenvector γ_{uv}.

(v) Take any cell V_u. Let λ'_{uv} denote the restriction of λ_{uv} to V_u. Then, the vectors λ'_{uv} for $v \in V(H) \setminus \{u\}$ can be interpreted as the first $\ell - 1$ columns of a $2^{\ell-2} \times 2^{\ell-2}$ Hadamard matrix M. We can assume that the last column of M is the all-ones vector. Let $\theta_1, ..., \theta_{2^{\ell-2}-\ell}$ be columns ℓ through $2^{\ell-2} - 1$ of M. Then, each θ_i is a ± 1 vector indexed by the vertices of V_u that assigns $+1$ to half of the vertices in any V_{uv}^j and -1 to the other half. Asserting that θ_i takes a value of 0 on all other cells, we see that each θ_i is an eigenvector with eigenvalue zero. There are $2^{\ell-2} - \ell$ such vectors for each vertex in H, for a multiplicity of $\ell(2^{\ell-2} - \ell)$.

It is easily confirmed that this is an orthogonal set of eigenvectors. Summing the multiplicities yields

$$1 + (\ell - 1) + \binom{\ell}{2} + \binom{\ell}{2} + \ell(2^{\ell-2} - \ell) = \ell \cdot 2^{\ell-2} = |V(G)|$$

so this is a complete set of eigenvectors. □

4.7.8 Corollary. *If $\ell = 4$, then G is a strongly regular graph.*

Proof. In this case, the multiplicity of the eigenvalue zero is $\ell(2^{\ell-2} - \ell) = 0$. Therefore, there are only three eigenvalues, and G is strongly regular. □

If $\ell = 4$, then G and $\mathcal{T}(G)$ are strongly regular graphs on 16 vertices, and are the smallest known pair of non-isomorphic cospectral strongly regular graphs.

4.7.9 Lemma. *For $\ell > 3k$, the graphs G and $\mathcal{T}(G)$ are k-equivalent.*

Proof. We will show that $H = K_\ell$ satisfies requirements of Theorem 4.7.6. For each $S_i \in \binom{V(H)}{3k}$, let v_i be any vertex not in S_i, and let e_i be any edge incident with v_i. Then, for any $S_i, S_j \in \binom{V(H)}{3k}$, the path consisting of e_i, (v_i, v_j) and e_j uses no edge contained in $S_i \cap S_j$. By Therefore, G and $\mathcal{T}(G)$ are k-equivalent. □

This gives us pairs of k-equivalent graphs for every k. Of course, this is trivial if G and $\mathcal{T}(G)$ are isomorphic.

4.7.10 Lemma. *For $H = K_\ell$, the graphs $G = G(H)$ and $\mathcal{T}(G)$ are not isomorphic.*

Proof. In order to prove this, we will show that G and $\mathcal{T}(G)$ have different clique numbers. In G, the vertices

$$C = \{(u, \mathbf{0}) \,:\, u \in V(H)\}$$

gives us a clique of size ℓ.

For the sake of concreteness, we will assume that $\mathcal{T}(G) = \mathcal{T}_{rs}(G)$; that is, the twist is applied at edge rs. If there is a clique $\mathcal{C}'$ of size ℓ in $\mathcal{T}_{rs}(G)$, then C' must contain exactly one vertex from each cell V_u. Let $((u, \mathbf{x}), (v, \mathbf{y}))$ be an edge of the clique C'. Then, if $\{u, v\} \neq \{r, s\}$, then $\mathbf{x}_{uv} + \mathbf{y}_{uv} = 0$. If $\{u, v\} = \{r, s\}$, then $\mathbf{x}_{uv} + \mathbf{y}_{uv} = 1$. Summing over the edges of C', we get

$$\sum_{((u,\mathbf{x}),(v,\mathbf{y}))\in E(C')} \mathbf{x}_{uv} + \mathbf{y}_{uv} = 1.$$

Recall that E_u denotes the set of edges incident at u in K_ℓ. We can rewrite the sum above as

$$\sum_{((u,\mathbf{x}),(v,\mathbf{y}))\in E(C')} \mathbf{x}_{uv} + \mathbf{y}_{uv} = \sum_{(u,\mathbf{x})\in C'} \sum_{e\in E_u} \mathbf{x}_e.$$

Since each vector $\mathbf{x}$ is of even weight, this sum must be zero. This gives a contradiction, so no such clique exists in $\mathcal{T}(G)$. □

We have shown that, if $H = K_\ell$ for $\ell > 3k$, then the graphs G and $\mathcal{T}(G)$ are non-isomorphic and k-equivalent. By Theorem 4.5.4, for $\ell > 3k$, we get a pair of graphs that are not distinguished by any k-particle invariant. The discussion in Section 4.5.1 tells us that this applies to the k-Boson invariant of Gamble et al. as well. By Theorem 4.6.6, if we take $\ell = 8$, we get a pair of non-isomorphic graphs on 512 vertices that are not distinguished by the discrete time walk invariant of Emms et al. It should be noted that these are not the only graphs known to defeat this invariant; Emms et al. [17] identify a pair of graphs with 14 vertices that are not distinguished.

Chapter 5

Jaeger Algebras

In this chapter, we will focus on two-particle quantum walks. The state of a two-particle walk on a graph $G = (V, E)$ is typically identified with a vector in $\mathbb{C}^V \otimes \mathbb{C}^V$. Instead, we will identify each two-particle state with an element of $\mathrm{Mat}_V(\mathbb{C})$, the set of $n \times n$ complex matrices whose rows and columns are indexed by V. This amounts to choosing the basis $\{e_u e_v^T : u, v \in V\}$ instead of the basis $\{e_u \otimes e_v : u, v \in V\}$. It is essentially a notational choice, but it will allow for a much more elegant presentation. Given an association scheme $\mathcal{A}$, the Jaeger algebra $\mathcal{J}_3$ is generated by the action of $\mathcal{A}$ on $\mathrm{Mat}_V(\mathbb{C})$ by left multiplication and Schur multiplication. The algebra $\mathcal{J}_4$ is generated by these actions, along with right multiplication. These algebras were first identified by Francois Jaeger, as recorded in his unpublished notes. The relevant page of these notes is reproduced in Section 5.5.4. For carefully chosen association schemes, the resulting Jaeger algebras provide a representation of the braid group, and therefore a method for constructing link invariants [31, 32]. The construction of these link invariants was Jaeger's original motivation for considering these algebras.

It is easy to verify that $\mathcal{J}_4$ contains the Hamiltonian for the two-particle continuous time quantum walk. We will show that $\mathcal{J}_4$ is semisimple and $\mathrm{Mat}_V(\mathbb{C})$ can be expressed as a sum of simple $\mathcal{J}_4$-modules. Our main objective in this chapter is to characterize the simple modules of $\mathcal{J}_4$. All results to this end are new.

A similar agenda has been undertaken by Caughman [10] and Curtin [14, 15] for Terwilliger algebras—equivalent to $\mathcal{J}_3$. However, many of the methods they employ will prove ineffective when applied to $\mathcal{J}_4$. Nonetheless, the work of Caughman and Curtin supplies us with many worthwhile questions about

$\mathcal{J}_4$.

In Section 5.5.2, we identify the simple $\mathcal{J}_4$-modules generated by diagonal matrices. We can associate one such module with each eigenvector of the underlying graph G. Moreover, in Theorem 5.5.9 we show that modules associated with the same eigenvalue are isomorphic.

In Section 5.5.3, we address the next natural class of $\mathcal{J}_4$-modules: those that are generated by matrices supported on the adjacency matrix of G. Lemma 5.5.3 states that a subset of the generators can be identified with the flow space of the graph G. If we restrict our attention to bipartite graphs, Theorem 5.5.17 gives us the remaining generators for these modules; they are associated with the symmetric counterpart to the flow space, which we refer to as the anti-flow space.

Finally, we present the simple $\mathcal{J}_4$ modules for the 4-cube, making use of the results proved throughout this section. In particular, apply Lemma 5.1.1, which guarantees a degree of symmetry in the $\mathcal{J}_4$-modules. This lemma is a surprising application of Corollary 3.1.33, which is concerned with strongly cospectral pairs of vertices. Although we consider only the 4-cube, the approach can be generalized to other graphs.

The two-particle walk takes place in a state space of dimension $|V|^2$. By decomposing this space into its simple $\mathcal{J}_4$-modules, we decompose the two-particle walk into a number of walks in much smaller spaces. This could allow us to parallelize the computation of the evolution of the two-particle walk; each of the smaller walks could be distributed to a different processor. Therefore, a general method for identifying the simple modules could have profound implications for the complexity of computing multi-particle walks. This chapter takes some of the first steps toward such a method.

5.1 Definitions

Let $\mathcal{A} = \{A_0, A_1, ..., A_d\}$ be a symmetric association scheme. For each $A_i \in \mathcal{A}$, we can define three endomorphisms of $\mathrm{Mat}_V(\mathbb{C})$:

$$
\begin{aligned}
X_i(M) &= A_i M \\
Y_i(M) &= M A_i \\
\Delta_i(M) &= A_i \circ M.
\end{aligned}
$$

We will now define a series of algebras generated by these operators. $\mathcal{J}_2$ is generated by

$$\{X_i : i = 0, ..., d\}.$$

$\mathcal{J}_3$ is generated by

$$\{X_i : i = 0, ..., d\} \cup \{\Delta_i : i = 0, ..., d\}.$$

Finally, $\mathcal{J}_4$ is generated by

$$\{X_i : i = 0, ..., d\} \cup \{Y_i : i = 0, ..., d\} \cup \{\Delta_i : i = 0, ..., d\}.$$

These algebras were first studied by Francois Jaeger in the context of spin models and representations of the braid group. This is where they got their numbering, as well as their name—*Jaeger algebras*.

Since both $\mathcal{J}_3$ and $\mathcal{J}_4$ are closed under adjoint, Lemma 2.2.3 tells us that $\mathcal{J}_3$ and $\mathcal{J}_4$ are semisimple algebras. Our primary aim in the rest of this chapter will be to identify and characterize the simple modules of $\mathcal{J}_3$ and $\mathcal{J}_4$.

If W is a $\mathcal{J}_k$-module. If $\mathcal{A}$ is P-polynomial, then the *endpoint* of W is the smallest value i such that

$$A_i \circ W \neq 0.$$

Similarly, if $\mathcal{A}$ is Q-polynomial and has idempotents $E_0, ..., E_\ell$, then the *dual-endpoint* j of W is the smallest value such that

$$E_i W \neq 0.$$

It will be convenient to classify $\mathcal{J}_k$-modules according to their endpoint.

If W is a $\mathcal{J}_k$-module, then its *stratification* is a vector $\mathbf{s} = \mathbf{s}(W)$ such that

$$\mathbf{s}_i = \dim(\Delta_i W).$$

5.1.1 Lemma. *Let G be a distance regular graph with strongly cospectral vertices u and v. Then, Moveover, if d is the diameter of G, then*

$$\Delta_i = X_d \Delta_{d-i} X_d, \qquad \Delta_i = Y_d \Delta_{d-i} Y_d$$

and, for any $\mathcal{J}_k$-module W with stratification $\mathbf{s} = \mathbf{s}(W)$,

$$\mathbf{s}_i = \mathbf{s}_{d-i}$$

for all i.

Proof. Lemma 3.1.33 tells us that the diameter of G is d and that A_d is an automorphism of G with $A_d^2 = I$. In this case,

$$X_d\Delta_i = \Delta_{d-i}X_d, \qquad Y_d\Delta_i = \Delta_{d-i}Y_d.$$

Therefore, if W is a $\mathcal{J}_k$-module, then X_d is an automorphism of W and

$$X_d(\Delta_i W) = \Delta_{d-i}W. \qquad \square$$

5.2 Triple Regularity

An association scheme $\mathcal{A} = \{A_0, .., A_\ell\}$ is *triply regular* if there are integers m_{ijk}^{rst} such that, for every u, v, w such that

$$(A_i)_{uv} = (A_j)_{vw} = (A_k)_{wu} = 1$$

there are exactly m_{ijk}^{rst} vertices x such that

$$(A_r)_{ux} = (A_s)_{vx} = (A_t)_{wx} = 1.$$

In other words, for all r, s, t and all vertices u, v, w,

$$\sum_{i,j,k} m_{ijk}^{rst}(A_i)_{uv}(A_j)_{vw}(A_k)_{wu} = \sum_{x\in V}(A_r)_{ux}(A_s)_{vx}(A_t)_{wx}.$$

Throughout this chapter, we will consider the Jaeger algebras of triply regular association schemes. The additional structure of triply regular schemes will allow us to say more about their Jaeger algebras than we can in the general case.

5.3 Terwilliger Algebras

Fix a vertex x in V. Then, we can define a series of diagonal matrices $F_i = F_i(x)$ such that

$$(F_i)_{yy} = (A_i)_{xy}.$$

That is, F_i acts like the identity on vertices y that are related to x by A_i. We refer to these matrices F_i as *dual idempotents*. The algebra generated by $A_0, ..., A_\ell$, along with $F_0, ..., F_\ell$ is known as the *Terwilliger algebra* relative to x, and is denoted by $\mathbb{T} = \mathbb{T}(x)$.

We can think of $\mathbb{T}$ as acting on the space of column vectors indexed by V. Consider the module generated by $\mathbf{1}$, the all-ones vector. It is spanned by the set $\{F_i\mathbf{1}\}$. The action of $\mathcal{A}$ on this module is given by

$$A_j(F_i\mathbf{1}) = \sum_k p_{ji}^k F_k\mathbf{1}.$$

This simple module is known as the *standard module*.

5.3.1 Lemma. *If W is the standard module, then $F_0W^\perp = 0$.*

Proof. Since

$$\dim(F_0(\mathrm{Mat}_V(\mathbb{C}))) = 1$$

and

$$\dim(F_0W) = 1$$

we must have $F_0W^\perp = 0$. □

We say that a $\mathbb{T}$-module W is *thin* if, for all F_i,

$$\dim(F_iW) \leq 1$$

and that it is *dual-thin* if, for all multiplicative idempotents E_i of $\mathcal{A}$,

$$\dim(E_iW) \leq 1.$$

A Terwilliger algebra is thin if all of its simple modules are thin. The following lemma is proven in [23]:

5.3.2 Lemma. *For any association scheme, and any vertex x, the standard module of $\mathbb{T}(x)$ is thin and dual-thin.*

Proof. Since it is spanned by $\{F_i\mathbf{1}\}$, the standard module W is thin. Therefore, if $\mathcal{A} = \{A_0, ..., A_\ell\}$, then $\dim(W) = \ell + 1$. Since $F_0\mathbf{1} = e_x$, we know that $E_ie_x \in W$ for all i. Since $\{E_ie_x : i = 0, ..., \ell\}$ is a set of $\ell + 1$ orthogonal vectors in W, it spans W. Since

$$E_jE_ie_x = \delta_{ij}E_ie_x$$

we have $\dim(E_jW) = 1$ for all j and the standard module is dual-thin. □

5.4 The Jaeger Algebra $\mathcal{J}_3$

While $\mathcal{J}_3$ has little significance in terms of multi-particle walks, it will give us some insight into the structure of $\mathcal{J}_4$, as well as providing a link to the theory of Terwilliger algebras. Given an association scheme $\mathcal{A}$, we will relate its Terwilliger algebras $\mathbb{T}(x_1), \ldots \mathbb{T}(x_n)$ to its Jaeger algebra $\mathcal{J}_3$. We begin with the following lemma:

5.4.1 Lemma. *Let S_i be the subspace of $Mat_V(\mathbb{C})$ made up of matrices that are zero everywhere except the i^{th} column. Then S_i is a $\mathcal{J}_3$-module.* □

Although the S_i are a set of orthogonal $\mathcal{J}_3$ modules, they are not, in general, simple. The following lemma can be found in [23],

5.4.2 Lemma. *The restriction of $\mathcal{J}_3$ to S_i is isomorphic to the Terwilliger algebra $\mathbb{T}(x_i)$.*

Proof. The isomorphism

$$\phi : \mathcal{J}_3|_{S_i} \to \mathbb{T}(x_i)$$

is given by

$$\phi(\Delta_j) \to F_j, \qquad \phi(X_j) \to A_j.$$ □

Therefore, the set of simple modules of $\mathcal{J}_3$ is the disjoint union of the simple modules for each of the Terwilliger algebras $\mathbb{T}(x_i)$. We will now show that, if $\mathcal{A}$ is triply regular, this has strong implications for the Terwilliger algebras $\mathbb{T}(x_i)$, and therefore for $\mathcal{J}_3$.

5.4.3 Lemma. *If $\mathcal{A}$ is a triply regular association scheme, then for each x, the Terwilliger algebra $\mathbb{T}(x)$ is completely determined by the values m_{ijk}^{rst}.*

Proof. First, note that the set $\{F_i A_j F_k\}$ forms a basis for the Terwilliger algebra $\mathbb{T}(x)$. Since

$$F_i A_j F_k \circ F_r A_s F_t = \delta_{ir}\delta_{js}\delta_{kt} \cdot F_i A_j F_k$$

this basis is orthogonal. Now, using triple regularity, we can calculate the product of two such basis elements:

$$(F_i A_s F_r)(F_q A_t F_k) = \delta_{rq} \sum_j m_{ijk}^{rst} \cdot F_i A_j F_k.$$

Therefore, the multiplicative structure of $\mathbb{T}(x)$ is completely determined by the values m_{ijk}^{rst}. □

5.4.4 Corollary. *If $\mathcal{A}$ is triply regular, then the Terwilliger algebras $\mathbb{T}(x_i)$ and $\mathbb{T}(x_j)$ are isomorphic, for all i, j.*

5.4.5 Corollary. *If $\mathcal{A}$ is triply regular, then $\mathcal{J}_3$ is determined, up to isomorphism, by the values m_{ijk}^{rst}.*

In particular, Corollary 5.4.5 tells us that, if $\mathcal{A}$ and $\mathcal{A}'$ are triply regular with the same parameters, then their Jaeger algebras $\mathcal{J}_3$ and $\mathcal{J}_3'$ are isomorphic. The following lemma was proven by Munemasa in a private communication:

5.4.6 Lemma. *If $\mathcal{A}$ is triply regular, then the operators $F_iA_jF_k$ are the basis relations of a cellular algebra.*

Proof. Let $W = \operatorname{span}\{F_iA_jF_k\}$. In the proof of Lemma 5.4.3, we saw that W is closed under Schur multiplication and matrix multiplication. We now observe that

$$(F_iA_jF_k)^T = F_kA_jF_i.$$

In addition,

$$I = \sum_i F_iA_0F_i, \qquad J = \sum_{ijk} F_iA_jF_k.$$

Thus, W is a cellular algebra. □

5.5 The Jaeger Algebra $\mathcal{J}_4$

We will now characterize some of the simple modules of $\mathcal{J}_4$. All of the results presented in this section are new. $\mathcal{J}_4$ is of particular interest, since it contains any 2-particle Hamiltonian of the form

$$H = M + N$$

where M is a movement term consisting of a sum of X_i and Y_i terms, corresponding to movement of the first and second particle respectively. The interaction term N consists of a sum of Δ_i terms.

A link between the modules of $\mathcal{J}_3$ and $\mathcal{J}_4$ is given by the following lemma:

5.5.1 Lemma. *A subspace W of $Mat_V(\mathbb{C})$ is a $\mathcal{J}_4$-module if and only if W and W^T are both $\mathcal{J}_3$-modules.*

Proof. The subspace W is a $\mathcal{J}_3$ module if and only if it is invariant under the action of X_i and Δ_i for all i. Similarly, if W^T is a $\mathcal{J}_3$-module, then it is invariant under X_i for all i. Equivalently, W is invariant under Y_i. Therefore, we know that W is a subspace of $\mathrm{Mat}_V(\mathbb{C})$ and is invariant under X_i, Y_i and Δ_i. Therefore, W is a $\mathcal{J}_4$-module. □

5.5.2 Corollary. *W is an simple $\mathcal{J}_4$-module if and only if W and W^T are simple $\mathcal{J}_3$-modules.*

5.5.3 Corollary. *If W is a $\mathcal{J}_3$-module and W is closed under transpose, then W is a $\mathcal{J}_4$-module. In particular, any $\mathcal{J}_3$ module spanned by symmetric and anti-symmetric matrices is a $\mathcal{J}_4$-module.*

5.5.4 Corollary. *If W is a $\mathcal{J}_4$-module containing a symmetric matrix, then $W = W^T$.*

5.5.1 The Standard Module of $\mathcal{J}_4$

Since $\mathcal{J}_4$ acts on the space of $n \times n$ matrices, we have a natural candidate for a $\mathcal{J}_4$-module—the Bose-Mesner algebra of $\mathcal{A}$. The action of $\mathcal{J}_4$ on $\mathrm{span}(\mathcal{A})$ is equivalent to $\mathcal{A}$ acting on itself by left, right, and Schur multiplication. Since an association scheme is closed under these operations, $\mathrm{span}(\mathcal{A})$ is clearly a $\mathcal{J}_4$-module.

To see that this module is simple, we note first that it is generated by the identity $I = A_0$. Now, for any $M \in \mathrm{span}(\mathcal{A})$, there is some i such that $\Delta_i(M) \neq 0$. Then,

$$\Delta_0 X_i(M) = \alpha A_0.$$

where α is non-zero. So A_0 is contained in the module generated by any M in $\mathrm{span}(\mathcal{A})$, and A_0 generates $\mathcal{A}$. Therefore, $\mathcal{A}$ is the basis of an simple $\mathcal{J}_4$ module. When referring to $\mathrm{span}(\mathcal{A})$ as a $\mathcal{J}_4$-module, we call it the *standard module.*

5.5.2 The Diagonal Modules of $\mathcal{J}_4$

In order to identify further simple modules with endpoint zero, we will assume that $\mathcal{A}$ is a triply regular association scheme. If $\mathbf{v}$ is a matrix indexed by V, then $D_{\mathbf{v}}$ will the matrix with $\mathbf{v}$ on the diagonal, and $W_{\mathbf{v}}$ will denote the

$\mathcal{J}_4$-module generated by $D_{\mathbf{v}}$. Let $\mathbb{T} = \mathbb{T}(x)$ be the Terwilliger algebra of $\mathcal{A}$ relative to x, and

$$F_0, ..., F_\ell = F_0(x), ..., F_\ell(x)$$

the dual idempotents relative to x.

We will begin by considering D_{e_x}—the matrix with a one in the xx entry and zeros elsewhere—and its corresponding module W_{e_x}. We will go on to identify a set of orthogonal, simple $\mathcal{J}_4$-modules.

5.5.5 Lemma. *If $\mathcal{A}$ is triply regular, then the non-zero elements of*

$$\{F_iA_jF_k :\ 0 \le i, j, k \le \ell\}$$

form a basis for W_{e_x}.

Proof. First, note that $W_{e_x} = F_0A_0F_0$. Now,

$$F_iA_jF_k = \Delta_j Y_j X_i(F_0A_0F_0).$$

Therefore, each matrix of this form is contained in the $\mathcal{J}_4$-module generated by W_{e_x}. We now verify that the span of these matrices is closed under the operations X_r, Y_r:

$$X_r(F_iA_jF_k) = \sum_{s,t} m_{stk}^{irj} F_sA_tF_k, \qquad Y_r(F_iA_jF_k) = \sum_{s,t} m_{its}^{kjr} F_iA_tF_s.$$

Now, we check for that $\operatorname{span}\{F_iA_jF_k\}$ is closed under Δ_r:

$$\Delta_r(F_iA_jF_k) = \delta_{rj}F_iA_jF_k.$$

Lastly, we note that the matrices are orthogonal:

$$F_iA_jF_k \circ F_rA_sF_t = \delta_{ir}\delta_{js}\delta_{kt}F_iA_JF_k. \qquad \square$$

Recall that the matrices $F_iA_jF_k$, which form a basis for W_{e_x} also form a basis for $\mathcal{T}(x)$, the Terwilliger algebra relative to x. Thus, the Terwilliger algebra relative to x is, in fact, a $\mathcal{J}_4$ module. What is more, since the action of $\mathcal{J}_4$ on this module is determined entirely by the triple regularity parameters m_{ijk}^{rst}, the modules W_{e_x} and W_{e_y} are isomorphic for all x, y. This is not surprising—Corollary 5.4.4 triple regularity guarantees that the Terwilliger algebras $\mathcal{T}(x)$ and $\mathcal{T}(y)$ are isomorphic. We can now state the following corollary to Lemma 5.5.5:

5.5.6 Corollary. *$W_{\mathbf{v}}$ is spanned by*

$$\mathcal{S}_{\mathbf{v}} = \left\{ \sum_x \mathbf{v}_x F_i(x) A_j F_k(x) : \; 0 \leq i, j, k \leq \ell \right\}. \qquad \square$$

Although $\mathcal{S}_{\mathbf{v}}$ spans $W_{\mathbf{v}}$, it may not be a basis. It is not, in general, linearly independent. In the proof of Lemma 5.5.5, we observed that the action of X_r, Y_r and Δ_r on the matrices $F_i A_j F_k$ is determined by the triple regularity parameters m_{ijk}^{rst}. By linearity, their action on the spanning set $\mathcal{S}_{\mathbf{v}}$ is also determined by these parameters.

Consider $\Delta_0(W_{\mathbf{v}})$, the elements of $W_{\mathbf{v}}$ that are non-zero only on the diagonal. This subspace is spanned by elements of the form

$$\sum_x \mathbf{v}_x F_i(x).$$

5.5.7 Lemma. *Let $\mathbf{v}$ be an eigenvector of the association scheme $\mathcal{A}$, and let p_i be such that $A_i \mathbf{v} = p_i \mathbf{v}$. Then,*

$$\sum_x \mathbf{v}_x F_i(x) = p_i D_{\mathbf{v}}.$$

Proof. Using the fact that $\mathbf{v}$ is an eigenvector, we can write

$$\begin{aligned} \sum_x \mathbf{v}_x F_i(x) &= \sum_{xy \in R_i} \mathbf{v}_x M_{yy} \\ &= \sum_y p_i \mathbf{v}_y M_{yy} \\ &= p_i D_{\mathbf{v}} \end{aligned}$$

as required. $\square$

Equivalently, $\Delta_0(W_{\mathbf{v}}) = \text{span}(D_{\mathbf{v}})$. We can now state the following new result, which characterizes the modules of endpoint zero.

5.5.8 Theorem. *Let $\{\mathbf{v}_1, ..., \mathbf{v}_n\}$ be an orthonormal set of eigenvectors for the association scheme $\mathcal{A}$. Then*

$$\{W_{\mathbf{v}_1}, ..., W_{\mathbf{v}_n}\}$$

is a set of orthogonal simple $\mathcal{J}_4$-modules.

Proof. To show that the modules are orthogonal, we will use the fact that $\mathcal{J}_4$ is closed under adjoint. We will take the inner product of arbitrary elements of $W_{\mathbf{v}_i}$ and $W_{\mathbf{v}_j}$. Take any K, L in $\mathcal{J}_4$. Then

$$\left\langle KD_{\mathbf{v}_i}, LD_{\mathbf{v}_j}\right\rangle = \left\langle D_{\mathbf{v}_i}, K^*LD_{\mathbf{v}_j}\right\rangle.$$

Since $D_{\mathbf{v}_i}$ is diagonal, we know that

$$\left\langle D_{\mathbf{v}_i}, K^*LD_{\mathbf{v}_j}\right\rangle = \left\langle D_{\mathbf{v}_i}, \Delta_0 K^*LD_{\mathbf{v}_j}\right\rangle.$$

Lemma 5.5.7 tells us that

$$\Delta_0 K^* L(D_{\mathbf{v}_j}) = \alpha \cdot D_{\mathbf{v}_j}$$

for some scalar α that depends on K and L. We can now rewrite our inner product as follows:

$$\begin{aligned}\left\langle KD_{\mathbf{v}_i}, LD_{\mathbf{v}_j}\right\rangle =& \left\langle D_{\mathbf{v}_i}, \alpha D_{\mathbf{v}_j}\right\rangle \\ =&\alpha \cdot \langle \mathbf{v}_i, \mathbf{v}_j\rangle \\ =&\alpha\delta_{ij}.\end{aligned}$$

Therefore, the modules $\{W_{\mathbf{v}_1}, ..., W_{\mathbf{v}_n}\}$ are orthogonal.

Take any $W_{\mathbf{v}_i}$, and assume that it is not simple. Since $\dim(\Delta_0 W_{\mathbf{v}_i}) = 1$, there must be some simple submodule W' of $W_{\mathbf{v}_i}$ such that $D_{\mathbf{v}_i} \in W'$. However, $D_{\mathbf{v}_i}$ generates $W_{\mathbf{v}_i}$, so $W' = W_{\mathbf{v}_i}$. Therefore, each $W_{\mathbf{v}_i}$ is simple. □

We refer to $\{W_{\mathbf{v}_1}, ..., W_{\mathbf{v}_n},\}$ as the *diagonal modules*. Note that the standard module is a diagonal module corresponding to the all-ones eigenvector.

5.5.9 Theorem. *Let* $\mathbf{v}$ *and* $\mathbf{u}$ *be eigenvectors of* $\mathcal{A}$ *such that, for all* i,

$$\mathbf{v}^* A_i \mathbf{v} = \mathbf{u}^* A_i \mathbf{u} = q_i.$$

Then $W_{\mathbf{v}}$ *and* $W_{\mathbf{u}}$ *are isomorphic as* $\mathcal{J}_4$*-modules.*

Proof. As we saw in Corollary 5.5.6, the module $W_{\mathbf{v}}$ is spanned by the set

$$\mathcal{S}_{\mathbf{v}} = \left\{\sum_x \mathbf{v}_x F_i(x) A_j F_k(x) :\ 0 \le i, j, k \le \ell\right\}$$

and $W_{\mathbf{u}}$ is spanned by an analogous set $\mathcal{S}_{\mathbf{u}}$. Define a mapping $\phi : W_{\mathbf{v}} \to W_{\mathbf{u}}$ as follows:

$$\phi\left(\sum_x \mathbf{v}_x F_i(x) A_j F_k(x)\right) = \sum_x \mathbf{u}_x F_i(x) A_j F_k(x).$$

We claim that ϕ is an isomorphism from $W_{\mathbf{v}}$ to $W_{\mathbf{u}}$. To prove this, we need to show that

(i) For any K in $\mathcal{J}_4$, the bijection ϕ commutes with K.

(ii) The bijection ϕ preserves inner products. Therefore, it is a linear bijection.

In the proof of Lemma 5.5.5, we saw that the action of $\mathcal{J}_4$ on $F_i(x)A_jF_k(x)$ is determined by the triple regularity parameters m_{ijk}^{rst}. Since elements of $\mathcal{S}_{\mathbf{v}}$ are linear combinations of these matrices, the action of $\mathcal{J}_4$ on $\mathcal{S}$ is also governed by the parameters m_{ijk}^{rst}. In particular, the weights $\mathbf{v}_x$ (resp.$\mathbf{u}_x$) are irrelevant to the action of $\mathcal{J}_4$ on $\mathcal{S}_{\mathbf{v}}$ (resp. $\mathcal{S}_{\mathbf{u}}$). Therefore, any $K \in \mathcal{J}_4$ commutes with ϕ.

We will now show that ϕ preserves inner products. Since $\mathcal{J}_4$ us closed under adjoint, this amounts to showing that, for any $K \in \mathcal{J}_4$

$$\langle D_{\mathbf{v}}, K(D_{\mathbf{v}})\rangle = \left\langle \phi\big(D_{\mathbf{v}}\big), \phi\big(K(D_{\mathbf{v}})\big)\right\rangle.$$

Since $\mathcal{J}_4$ acts identically on $\mathcal{S}_{\mathbf{v}}$ and $\mathcal{S}_{\mathbf{u}}$, we can simplify this further, requiring only that

$$\left\langle D_{\mathbf{v}}, \sum_x \mathbf{v}_x F_i(x) A_j F_k(x)\right\rangle = \left\langle D_{\mathbf{u}}, \sum_x \mathbf{u}_x F_i(x) A_j F_k(x)\right\rangle$$

for all i, j, k. If $j \neq 0$ or $i \neq k$, both sides of this equation are zero. Thus, we need only consider

$$\left\langle D_{\mathbf{v}}, \sum_x \mathbf{v}_x (F_i(x))\right\rangle = \langle D_{\mathbf{v}}, q_i D_{\mathbf{v}}\rangle = q_i.$$

An analogous calculation gives the same value for $\mathbf{u}$.

Since ϕ preserves inner products it is a linear bijection. Together with the fact that ϕ commutes with $\mathcal{J}_4$, this implies that ϕ is an isomorphism from $W_{\mathbf{v}}$ to $W_{\mathbf{u}}$. □

We now have a complete set of orthogonal simple $\mathcal{J}_4$-modules of endpoint zero. We might hope that these modules are also thin, but the following lemma shows that this is not the case.

5.5.10 Lemma. *If* $\mathbf{v}$ *is an eigenvector, then the diagonal module* $W_{\mathbf{v}}$ *is not thin unless either*

(i) $\mathbf{v} = k\mathbf{1}$*, a constant vector.*

(ii) The association scheme $\mathcal{A}$ *is bipartite with partition* $\{V_1, V_2\}$ *and* $\mathbf{v}$ *takes the value* $+k$ *on* V_1 *and* $-k$ *on* V_2 *for some* k*.*

Proof. If $W_{\mathbf{v}}$ is thin, then $\dim(\Delta_i(W_{\mathbf{v}})) \leq 1$ for all i. In particular, we must have

$$X_i(D_{\mathbf{v}}) = \alpha_i Y_i(D_{\mathbf{v}})$$

for some scalar Y. Let x, y be vertices such that $(A_i)_{xy} = 1$. Then,

$$X_i(D_{\mathbf{v}})_{yx} = \mathbf{v}_x, \qquad X_i(D_{\mathbf{v}})_{xy} = \mathbf{v}_y.$$

Similarly,

$$Y_i(D_{\mathbf{v}})_{yx} = \mathbf{v}_y, \qquad Y_i(D_{\mathbf{v}})_{xy} = \mathbf{v}_x.$$

This gives us two equations:

$$\mathbf{v}_x = \alpha_i \mathbf{v}_y, \qquad \mathbf{v}_y = \alpha_i \mathbf{v}_x.$$

Therefore, $\alpha_i = \pm 1$ for all i. This leaves us with two possibilities:

(i) If $\alpha_i = 1$ for all i, then $\mathbf{v}$ is a multiple of the all-ones vector.

(ii) Otherwise, the entries of $\mathbf{v}$ contain only two values, $\pm k$, defining a bipartition of V. Each A_i relates vertices within the partitions ($\alpha_i = 1$) or vertices in opposite partitions ($\alpha_i = -1$). In this case, $\mathcal{A}$ is bipartite, and $\mathbf{v}$ identifies the bipartition. □

5.5.3 Modules with Endpoint One

In the previous section, we identified the diagonal modules—a complete set of simple modules of endpoint zero. Let $\mathcal{W}_k$ denote the sum of modules of endpoint k. We would like to characterize its orthogonal complement $\mathcal{W}_0^{\perp}$.

We can immediately observe that any M in $\mathcal{W}_0^\perp$ must have rows and columns summing to zero since

$$\langle D_{e_u}, JM\rangle = \langle D_{e_u}, MJ\rangle = 0.$$

Recall that $\mathcal{W}_0$ was spanned by elements of the form

$$F_i(x)A_jF_k(x).$$

Therefore, $\mathcal{W}_0^\perp$ consists of all matrices M satisfying

$$\langle F_i(x)A_jF_k(x), M\rangle = 0$$

for all i, j, k and x. Setting $j = 1$ gives us the following lemma:

5.5.11 Lemma. *The direct sum of all modules of endpoint one, denoted by $\mathcal{W}_1$ is generated by the set of matrices M such that $\Delta_1(M) = M$ and*

$$\langle F_i(x)A_1F_k(x), M\rangle = 0$$

for all i, k and x. □

Our objective will be to identify generators for simple submodules of $\mathcal{W}_1$. That is, we will characterize the matrices M with $\Delta_1(M) = M$,

$$\langle F_i(x)A_1F_k(x), M\rangle = 0$$

for all i, k and x, and M generates a simple $\mathcal{J}_4$ module. In general, finding such generators M is difficult; we will focus on the case when $\mathcal{A}$ is the association scheme of a distance regular graph G.

We now introduce the notion of a *cut* of a graph. Given a partition (V_1, V_2) of the vertices of G, we associate with it a function

$$c : V \times V \to \{0, 1\}$$

such that

$$c(u, v) = \begin{cases} 1 & u \in V_1,\ v \in V_2,\ uv \in E(G) \\ 0 & \text{otherwise.} \end{cases}$$

With any cut c, we associate a matrix M_c such that

$$(M_c)_{uv} = c(u, v).$$

We call the span of all such cut matrices the *cut space* of the graph G.

5.5.12 Lemma. *Let G be a distance regular graph and set*

$$M = F_i(x)A_1F_k(x)$$

for some i, j and vertex x. Then, $M = M_c$, the matrix corresponding to a cut $c = c(x; i, k)$. □

As a consequence of Lemmas 5.5.11 and 5.5.12, the module $\mathcal{W}_1$ is generated by matrices orthogonal to cut matrices M_c for $c = c(x; j, k)$. We will proceed by trying to characterize this orthogonal complement.

We will focus on two cases—when M is anti-symmetric and when it is symmetric. We will show that all antisymmetric matrices M satisfying Lemma 5.5.11 can be identified with a *flow* on the graph G. A flow is a function

$$f : V \times V \to \mathbb{C}$$

such that

(i) If $uv \notin E$, then $f(u, v) = 0$.

(ii) The function f is antisymmetric: $f(u, v) = -f(v, u)$.

(iii) For each v in V, we have $\sum_{u \in V} f(u, v) = 0$.

To any flow f, we can assign a *flow matrix* M_f such that

$$(M_f)_{uv} = f(u, v).$$

Note that the requirements (i)-(iii) are equivalent to

(i) $\Delta_1(M_f) = M_f$

(ii) M is antisymmetric.

(iii) The columns (and therefore rows) of M sum to zero.

The span of the flow matrices is the known as the *flow space* of G. Let $r = v_0, v_1, ..., v_k$ be a cycle in G with $v_0 = v_k$. Then, we can define a flow f_r with $f_r(v_i, v_{i+1}) = 1$ and $f_r(v_i, v_{i-1}) = -1$. We will make use of the following well-known lemmas (see, for example, [29], Chapter 14):

5.5.13 Lemma. *There is a subset C of the cycles in G such that*

$$\{M_{f_r} : r \in C\}$$

forms a basis for the flow space of G. □

5.5.14 Lemma. *In the subspace $\Delta_1(Mat_V(\mathbb{C}))$, the cut space is the orthogonal complement of the flow space.* □

Therefore, the antisymmetric subspace of $\Delta_1(\mathcal{W}_1)$ is a subspace of the flow space of G. Conversely, and antisymmetric matrix in $\Delta_1(\mathcal{W}_1)$ must satisfy the requirements (i)-(iii) above, and can therefore be associated with a flow. This gives us the following lemma:

5.5.15 Lemma. *The antisymmetric subspace of $\Delta_1(\mathcal{W}_1)$ is the flow space of G.* □

We now consider the symmetric case. An *anti-flow* is a function

$$a : V \times V : \mathbb{C}$$

such that

(i) If $uv \notin E$, then $f(u,v) = 0$.

(ii) The function f is symmetric: $f(u,v) = f(v,u)$.

(iii) For each v in V, we have $\sum_{u \in V} f(u,v) = 0$.

Just as we did with flows, we associate a matrix M_a with the anti-flow a:

$$(M_a)_{uv} = a(u,v).$$

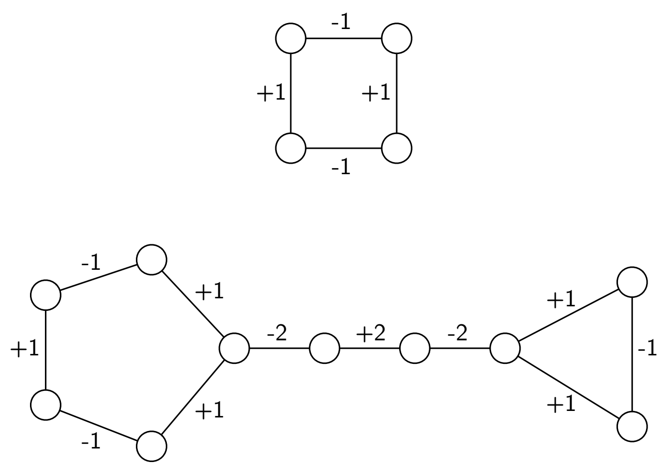
Any anti-flow matrix M_a can be associated with a weighted graph G_a, which is a subgraph of G. The span of the matrices M_a is the *anti-flow* space of G. For any symmetric M in $\Delta_1(\mathcal{W}_1)$, we have $M = M_a$ for some anti-flow a. Theferore, $\Delta_1(\mathcal{W}_1)$ is a subspace of the anti-flow space. The following theorem, proved by Akbari, Ghareghani, Khosrovshahi, and Maimani in [1] describes a set of basis elements for the anti-flow space:

5.5.16 Theorem. *The anti-flow space for a graph G has a basis of matrices M_a such that each G_a is described by one of the following:*

1. *An even cycle in G, with weights $+1$ and -1 assigned alternately to the edges of the cycle.*

2. *Two disjoint odd cycles r_1 and r_2 joined by a path that meets r_1 at u and r_2 at v. The weights $+1$ and -1 are assigned alternately to the vertices of r_1, beginning at u. The values $+2$ and -2 are assigned alternately to the edges of the path. Finally, the values $+1$ and -1 are assigned alternately to r_2, starting at v.* □

Figure 5.5.1: Examples of the weighted subgraphs that span the anti-flow space.



These two types of subgraphs are illustrated in Figure 5.5.1. Note that, since a bipartite graph contains no odd cycles, its anti-flow space is spanned by weighted subgraphs of the first type only. If r is an even cycle in G, let a_r denote the anti-flow obtained by assigning ± 1 alternately to its edges.

Then, we have the following theorem:

5.5.17 Theorem. *If G is bipartite, then the there is a set of cycles C such that the module $\mathcal{W}_1$ is generated by*

$$\{M_{f_r} : r \in C\} \cup \{M_{a_r} : r \in C\}. \qquad \square$$

The set C is a basis for the *cycle space* of G. It is well-known that, if G is connected,

$$|C| = |E| - |V| + 1.$$

See, for example, [16], Chapter 1. This gives the following corollary:

5.5.18 Corollary. *Let G be a bipartite graph. Then,*

$$\dim(\Delta_1 \mathcal{W}_1) = 2(|E| - |V| + 1). \qquad \square$$

Since the M_{f_r} are symmetric and the M_{a_r} are antisymmetric, they are orthogonal to each other. Note that, although Theorem 5.5.17 gives us a set of generators, it does not, in general, tell us how to identify generators for *simple* modules.

Example: The Simple Modules of the 4-Cube

We will now consider the simple $\mathcal{J}_4$-modules of the 4-cube. The 4-cube $Q_4 = (V, E)$ has vertex set $\mathbb{Z}^4$. Two vertices are adjacent if they differ in exactly one place. It is a distance regular graph on 16 vertices, with 32 edges and diameter 4. It is also easily verified that it is triply regular. Let A_i denote the distance i adjacency matrix. Vertices at distance 4 are strongly cospectral, so appealing to Lemma 5.1.1, we know that the stratification $\mathbf{s}$ of any $\mathcal{J}_4$-module will have $\mathbf{s}_i = \mathbf{s}_{4-i}$. We begin with a summary of the structure of the simple $\mathcal{J}_4$ modules. We will then give the details of the lemmas and computations that allow us to characterize these modules.

We begin with the diagonal modules. The spectrum of Q_4 is

$$((-4)^1, (-2)^4, 0^6, 2^4, 4^1).$$

Since the diagonal modules associated with each eigenvalue $p(i)$ are isomorphic, they have the same stratification $\mathbf{s}^0_{p(i)}$. Computationally, we find that

$$\begin{aligned} \mathbf{s}^0_4 = \mathbf{s}^0_{-4} =& (1, 1, 1, 1, 1) \\ \mathbf{s}^0_2 = \mathbf{s}^0_{-2} =& (1, 2, 2, 2, 1) \\ \mathbf{s}^0_0 =& (1, 2, 3, 2, 1). \end{aligned}$$

Taking into account multiplicities and summing, we get the stratification $\mathbf{s}(\mathcal{W}_0)$ of $\mathcal{W}_0$:

$$\mathbf{s}(\mathcal{W}_0) = (16, 30, 36, 30, 16).$$

In particular, we note that $\dim(\Delta_1 \mathcal{W}_0) = 30$. Since A_1 has 64 non-zero entries, we expect that $\dim(\Delta_1 \mathcal{W}_1) = 34$. This agrees with Corollary 5.5.18.

The simple modules of endpoint one have two stratifications:

$$\begin{aligned} \mathbf{s}^1_1 =& (0, 1, 2, 1, 0) \\ \mathbf{s}^1_{-1} =& (0, 1, 1, 1, 0) \end{aligned}$$

There are 16 simple modules with the stratification $\mathbf{s}^1_1$ and 18 modules with the stratification $\mathbf{s}^1_{-1}$. This gives us

$$\mathbf{s}(\mathcal{W}_0) = (0, 34, 50, 34, 0).$$

Summing the stratification of $\mathcal{W}_0$ and $\mathcal{W}_1$, we get

$$\mathbf{s}(\mathcal{W}_0 + \mathcal{W}_1) = (16, 64, 86, 64, 16).$$

Since A_2 has 96 non-zero entries, this means $\dim(\mathcal{W}_2) = 10$. Since G is bipartite, this also means that every module with endpoint two is one-dimensional:

$$\mathbf{s}_0^2 = (0, 0, 1, 0, 0).$$

These modules and their stratifications are presented graphically in Figure 5.5.2.

We will now describe the simple modules with endpoint one in detail. The symmetry guaranteed by Lemma 5.1.1 will allow us to identify some criteria for these modules. We begin with the following simple lemma:

5.5.19 Lemma. *Any element B of $\mathcal{J}_4$ for the 4-cube can be written as a sum*

$$B = \sum_i T_i$$

where each T_i is a product of elements of the form $\Delta_j X_1 \Delta_k$ or $\Delta_j Y_1 \Delta_k$.

Proof. This is a consequence of the definition of $\mathcal{J}_4$ and the observation that $\sum_j \Delta_j = I$. □

Now, applying Lemma 5.1.1, we have

$$\Delta_4 = X_4 \Delta_0 X_4, \qquad \Delta_3 = X_4 \Delta_1 X_4.$$

If W is a $\mathcal{J}_4$-module with endpoint one, we can disregard Δ_0. We also note that

$$\Delta_j X_1 \Delta_j = \Delta_j Y_1 \Delta_j = 0.$$

Combining these observations with Lemma 5.5.19 gives the following corollary:

5.5.20 Corollary. *If W is a $\mathcal{J}_4$ module of the 4-cube with endpoint one, then any element B of $\Delta_1 \mathcal{J}_4 \Delta_1$ acting on $\Delta_1 W$ can be written as a sum of elements of the set*

$$\{\Delta_1 X_1 X_1 \Delta_1,\ \Delta_1 Y_1 Y_1 \Delta_1,\ \Delta_1 X_1 Y_1 \Delta_1\}.$$

Proof. We know that each T_i is a product of elements of the set

$$\mathcal{S} = \{\Delta_1 X_1 \Delta_2,\ \Delta_2 X_1 \Delta_1,\ \Delta_1 Y_1 \Delta_2,\ \Delta_2 Y_1 \Delta_1,\}.$$

Calculating the pairwise products of this set and noting that any element of $\Delta_1 \mathcal{J}_4 \Delta_1$ must start and end with Δ_1 gives us the Corollary. □

We will now identify the generators of the modules with endpoint one. We begin with the symmetric ones—those identified with anti-flows—and then use these to construct the anti-symmetric ones. Note that each element of $\mathcal{S}$ is a symmetric linear operator on $\Delta_1 \mathcal{W}_1$. Therefore, each can be associated with an orthogonal set of eigenvectors that form a basis of $\Delta_1 \mathcal{W}_1$. Moreover, if M is a common eigenvector of each element of $\mathcal{S}$, then it generates a simple $\mathcal{J}_4$ module W with $\dim(\Delta_1(W)) = 1$. Our goal is to identify these common eigenvectors.

Any anti-flow on the 4-cube is an eigenvector of $\Delta_1 X_1 X_1 \Delta_1$ and $\Delta_1 Y_1 Y_1 \Delta_1$ with eigenvalue one in each case. Therefore, we are looking for anti-flows that are eigenvectors of $\Delta_1 X_1 Y_1 \Delta_1$. It is easily verified that the cycle space of the 4-cube has a basis C consisting only of 4-cycles. Theorem 5.5.17, tells us that the anti-flows associated with C span the anti-flow space. Now, the action of $\Delta_1 X_1 Y_1 \Delta_1$ on the set of 4-cycles is linear, symmetric and non-singular. Therefore, it must have a set of eigenvectors that form a basis for the anti-flow space of the 4-cube. In particular, we can expect each simple $\mathcal{J}_4$-module W of endpoint one to satisfy $\dim \Delta_1(W) = 1$.

Computationally, we find that $\Delta_1 X_1 Y_1 \Delta_1$ has eigenvalues 1, -1 and 3 when acting on the anti-flow space of the 4-cube, with multiplicities 8,6 and 3. The resulting modules have stratification $(0, 1, 2, 1, 0)$, $(0, 1, 1, 1, 0)$ and $(0, 1, 1, 1, 0)$, respectively.

We will now identify the corresponding anti-symmetric generators. Since G is bipartite, any matrix M in $\Delta_1 \mathcal{W}_1 \cup \Delta_3 \mathcal{W}_1$ can be written in the form

$$M = \begin{pmatrix} 0 & D \\ D^T & 0 \end{pmatrix}$$

for some matrix D. Any matrix L in $\Delta_2 \mathcal{W}_1$ can be written as

$$L = \begin{pmatrix} R & 0 \\ 0 & S \end{pmatrix}$$

Let Z be the operator defined by

$$Z\begin{pmatrix}0 & D\\ D^T & 0\end{pmatrix} = \begin{pmatrix}0 & D\\ -D^T & 0\end{pmatrix}$$
$$Z\begin{pmatrix}R & 0\\ 0 & S\end{pmatrix} = \begin{pmatrix}-R & 0\\ 0 & S\end{pmatrix}.$$

Z commutes with X_1 and Δ_i for all i. It anti-commutes with Y_1. Therefore, if W is a simple module with endpoint one generated by a symmetric matrix M, ZW is an orthogonal simple module with endpoint one generated by the antisymmetric matrix ZM. Moreover, ZW has the same stratification as W. If M_1 and M_2 are orthogonal matrices, then ZM_1 and ZM_2 are orthogonal. Therefore, if $\{W_i : 1 \leq i \leq 17\}$ is an orthogonal set of simple $\mathcal{J}_4$-modules generated by the anti-flows on the 4-cube, then

$$\{W_i : 1 \leq i \leq 17\} \cup \{ZW_i : 1 \leq i \leq 17\}$$

is a complete orthogonal set of simple $\mathcal{J}_4$-modules with endpoint one.

5.5.4 A note from Francois Jaeger

Below is a page of Francois Jaeger's unpublished notes from a lecture he gave at the 1993 International Conference on Algebraic Combinatorics in Fukuoka, Japan. The notes were part of his correspondence with Chris Godsil. They contain the first mention of the algebras that bear his name in this thesis.

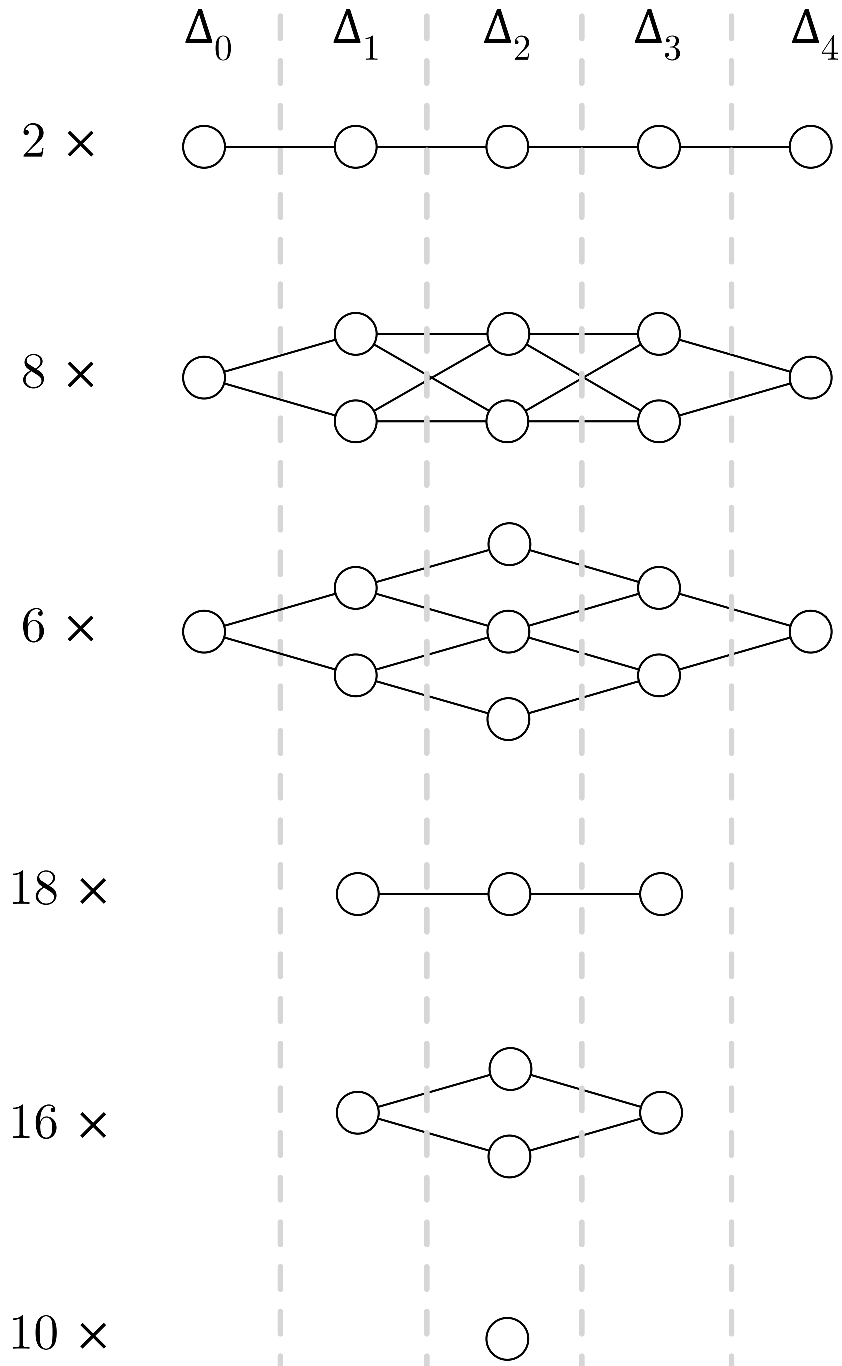
Remark : The graphs needed for Kauffman, $a = -t^5$, "contain" the square designs needed for Homfly, $a = t^4$.

Remark : A spin model representation of $\mathcal{C}_3(a,t)$ is exactly Terwilliger's algebra of the corresponding strongly regular graph. What about $\mathcal{C}_k(a,t)$ $\forall k$?

This leads us to consider for any association scheme $(X, A_i, i=0,..d)$ an algebra of endomorphisms of $V \otimes --- \otimes V$ (where V has basis X) for any number of factors. Each element A of the Bose Mesner algebra would act on each V in the standard way, and on each pair of consecutive V's diagonally.

The structure of this algebra would be particularly interesting for triply regular schemes.

Figure 5.5.2: The stratification of the simple $\mathcal{J}_4$-modules for the 4-cube.



Chapter 6

Future Work

In this chapter, we will outline some directions for future work. This discussion will be organized in the same way as the thesis: we will begin with single particle quantum walks, proceed to cellular algebras and graph invariants, and conclude with Jaeger algebras.

While periodicity and perfect state transfer are relatively well understood, pretty good state transfer remains somewhat elusive. While we identified sufficient conditions for pretty good state transfer in Theorem 3.1.19, these conditions are far from necessary. A more precise characterization of pretty good state transfer would be very useful.

Pretty good state transfer takes place in the path on n vertices if and only if $n+1$ is a prime, twice a prime, or a power of two. Therefore, an efficient test for pretty good state transfer on the path is equivalent to a test for primality. We would also like to establish a bound $f(G,u,v)$ such that, if there is no pretty good state transfer from u to v, then

$$|e_u^T U(t) e_v| < f(G,u,v).$$

A time t at which the inequality is violated serves as a certificate for pretty good state transfer. In the case of the path, such a time t could serve as a certificate for primality. Of course, it is not clear that such a certificate could be efficiently verified.

In Chapter 4, we showed that pairs of k-equivalent graphs are not distinguished by the invariants of Emms et al. and Gamble et al. We described a construction for pairs of non-isomorphic k-equivalent graphs. There are two ways that these constructions could be improved. The graphs have diameter two and four eigenvalues. In this sense, they are "nearly" strongly regular.

We would like to find a similar construction for strongly regular graphs. This would resolve the conjecture of Emms at al. that their invariant distinguishes all strongly regular graphs. It would also be nice to find smaller examples that exhibit the same degree of regularity. For example, our construction for two-equivalent graphs is on 512 vertices. What is worse, the number of vertices grows exponentially with k. Both Gamble et al. and Emms et al. have suggested that their invariants may be strong enough to distinguish all strongly regular graphs. Therefore, a construction for strongly regular pairs of non-isomorphic k-equivalent graphs would be particularly interesting.

It would be useful to place a lower bound on the size of non-isomorphic k-equivalent graphs. Put another way, for any n, let $g(n)$ be the smallest value such that there are no non-isomorphic pairs of $g(n)$-equivalent graphs on at most n vertices. Then, any algorithm that tests for $g(n)$-equivalence also tests for isomorphism on graphs of size n. The Weisfeiler-Lehman algorithm of degree $3g(n)$ is such a test. On graphs with n vertices, its running time is polynomial in $n^{g(n)}$. Therefore, an upper bound on $g(n)$ could yield a faster algorithm for the graph isomorphism problem. Note that we already know that $g(n)$ cannot be constant, so this approach will not yield a polynomial-time algorithm.

In Chapter 5, we introduced the Jaeger algebras. Our main objective was to characterize the simple $\mathcal{J}_4$-modules for triply regular graphs. We presented a method for generating modules of endpoint zero. We made some progress with modules of endpoint one, particularly in the case of bipartite graphs. It would be nice to have a more general method for generating these modules, as well as those with endpoint greater than one.

The decomposition of $\mathrm{Mat}_V(\mathbb{C})$ into simple $\mathcal{J}_4$ modules has computational implications as well. It divides the two-particle walk into a number of smaller walks. Computing the evolution of these component parts can then be distributed among several processors. It would be very interesting to formalize this process and examine its efficacy.

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