

Symmetric Squares of Graphs

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Abstract

We consider *symmetric powers* of a graph. In particular, we show that the spectra of the symmetric square of strongly regular graphs with the same parameters are equal. We also provide some bounds on the spectra of the symmetric squares of more general graphs. The connection with generic exchange Hamiltonians in quantum mechanics is discussed in an appendix.

1 Introduction

The *symmetric k -th power* $X^{\{k\}}$ of a graph X is constructed as follows: its vertices are the k -subsets of $V(X)$, and two k -subsets are adjacent if and only if their symmetric difference is an edge. As an example, and a test case, the symmetric square of the complete graph K_n is its line graph. (Useful procedures for constructing symmetric squares of arbitrary graphs will be given in Theorem 4.1 and Lemma 9.1). Symmetric powers were introduced in [1].

The symmetric powers are related to a class of random walks, where one starts with k particles occupying k distinct vertices of X , and, at each step of the walk, a single particle moves to an unoccupied adjacent site. More formally, we can generalise the concept of a walk on a graph to a k -walk, which is an alternating sequence of k -subsets of vertices V_i and arcs e_i , $(V_0, e_1, V_1, e_2 \dots, e_n, V_n)$, such that the symmetric difference of V_{i-1} and V_i is the arc e_i . It is readily seen that a k -walk on X corresponds to an ordinary 1-walk on $X^{\{k\}}$.

Our motivation for studying symmetric powers arises from its relevance for physically realisable systems and for the graph isomorphism problem. A brief outline of the connection between symmetric powers and exchange Hamiltonians in quantum mechanics is given in the appendix.

The relevance to the graph isomorphism problem arises because invariants of the symmetric powers of X are invariants of X . There are examples of cospectral graphs X and Y such that $X^{\{2\}}$ and $Y^{\{2\}}$ are not cospectral. In fact we have verified computationally that graphs on at most 10 vertices determined by the spectra of their symmetric squares. On the other hand, the main result of this

paper is a proof that if X and Y are cospectral strongly-regular graphs then $X^{\{2\}}$ and $Y^{\{2\}}$ are cospectral. There is also a family of five regular graphs on 24 vertices whose symmetric squares are cospectral. Nevertheless, in each of those cases, and, in fact, for all graphs we have examined (including strongly regular graphs on up to 36 vertices), the spectrum of the symmetric *cubes* determine the original graphs. (The computations on the the strongly regular graphs on 35 and 36 vertices were performed by Dumas, Pernet and Saunders; more details are given in Section 10.)

If it were true for some fixed k that any two graphs X and Y are isomorphic if and only if their k -th symmetric powers are cospectral, then we would have a polynomial-time algorithm for solving the graph isomorphism problem. For a pessimist this suggests that, for each fixed k , there should be infinitely many pairs of non-isomorphic graphs X and Y such that $X^{\{k\}}$ and $Y^{\{k\}}$ are cospectral.

In the last section of the paper we will consider bounds, from an algebraic perspective, on the spectra of the symmetric squares of arbitrary graphs.

While the focus of this paper is on the spectra of the symmetric squares, it should be noted that multivalued graph invariants based on generic (analytic) matrix valued functions $f(A^{\{k\}})$ can also be considered [1], where $A^{\{k\}}$ is the adjacency matrix of $X^{\{k\}}$. In [2] this approach was followed, and numerical computations showed that the values of $\exp(iA^{\{2\}})$ sufficed to distinguish all strongly regular graphs up to around 30 vertices.

2 Preliminaries

If A is square matrix, then let $\phi(A, t)$ denote the characteristic polynomial $\det(t\mathbb{I} - A)$ of A . If A is the adjacency matrix of X , we will also write $\phi(X, t)$. If x and y are vertices of X , we write $x \sim y$ to denote that x is adjacent to y .

A graph is *strongly regular* with parameters $(v, k; a, c)$ if it is not complete or empty, has v vertices, and the number of common neighbours of two vertices x and y is k , a or c according as x and y are equal, adjacent, or distinct and not adjacent. Thus if X is strongly regular, the neighbourhood of each vertex in X is regular and the neighbourhood of each vertex in the complement of X is regular. The line graph of the complete graph K_n is strongly regular if $n \geq 3$.

The main tool in this paper will be walk-generating functions. If A is the adjacency matrix of the graph X , then the walk-generating function $W(X, t)$ is the formal power series

$$\sum_{r \geq 0} A^r t^r.$$

We view this either as a power series with coefficients from the ring of matrices, or as a matrix whose entries are power series over \mathbb{R} . Its ij -entry $W_{i,j}(X, t)$ is the generating function for the walks in X that start at the vertex i and finish at j .

If $D \subseteq V(G)$, then $W_{D,D}(X, t)$ denotes the submatrix of $W(X, t)$ with rows and columns indexed by the vertices in D . The following identities are proved in Chapter 4 of [3].

2.1 Theorem. *If D is a subset of d vertices of X , then*

$$t^{-d} \det(W_{D,D}(X, t^{-1})) = \frac{\phi(X \setminus D, t)}{\phi(X, t)}. \quad \square$$

2.2 Corollary. *If $i \in V(X)$, then*

$$t^{-1} W_{i,i}(X, t^{-1}) = \frac{\phi(X \setminus i, t)}{\phi(X, t)}. \quad \square$$

2.3 Corollary. *If i and j are distinct vertices of X ,*

$$t^{-1} W_{i,j}(X, t^{-1}) = \frac{(\phi(X \setminus i, t)\phi(X \setminus j, t) - \phi(X, t)\phi(X \setminus ij, t))^{1/2}}{\phi(X, t)}. \quad \square$$

The presence of the square root in the previous identity is surprising. Note though that it causes no ambiguity, since we know that the coefficients of $W_{i,j}(G, t)$ are non-negative.

We apply these identities to obtain information about strongly regular graphs. If X is strongly regular with parameters $(v, k; a, c)$ and adjacency matrix A then

$$A^2 - (a - c)A - (k - c)\mathbb{I} = c\mathbb{J}.$$

(This is essentially the definition of “strongly regular” expressed in linear algebra.) Since X is regular A and \mathbb{J} commute, whence we see that for each non-negative integer k , the power A^k is a linear combination of \mathbb{I} , \mathbb{J} and A . Thus the generating function $W_{i,j}(X, t)$ depends only on whether the vertices i and j are equal, adjacent, or distinct and not adjacent. Using the corollaries above, this leads to the following:

2.4 Theorem. *Let X be a strongly regular graph. Then $\phi(X \setminus i, t)$ is independent of i and, if $i \neq j$, then $\phi(X \setminus ij, t)$ only depends on whether i and j are adjacent or not.* \square

2.5 Theorem. *Let X be a strongly regular graph and let D_1 and D_2 be induced subgraphs of $V(X)$. If D_1 and D_2 are cospectral with cospectral complements, then $X \setminus D_1$ and $X \setminus D_2$ are cospectral with cospectral complements.*

Proof. Suppose $D \subseteq V(X)$. Then $W_{D,D}(X, t)$ is the submatrix of $W(X, t)$ with rows and columns indexed by the vertices in D . Since X is strongly regular, we have

$$W_{D,D}(X, t) = \alpha\mathbb{I} + \beta\mathbb{J} + \gamma A(D)$$

where α , β and γ are generating functions and $A(D)$ is the adjacency matrix of the subgraph induced by D . So

$$\begin{aligned} \det(\alpha\mathbb{I} + \beta\mathbb{J} + \gamma A(D)) &= \det((\alpha\mathbb{I} + \gamma A(D))(\mathbb{I} + (\alpha\mathbb{I} + \gamma A(D))^{-1}\beta\mathbb{J})) \\ &= \det(\alpha\mathbb{I} + \gamma A(D)) \det(\mathbb{I} + (\alpha\mathbb{I} + \gamma A(D))^{-1}\beta\mathbb{J}) \end{aligned}$$

Recall that if the matrix products BC and CB are defined then

$$\det(\mathbb{I} + BC) = \det(\mathbb{I} + CB).$$

Since

$$= \det(\mathbb{I} + (a\mathbb{I} + cA(D))^{-1}b\mathbf{1}\mathbf{1}^T)\mathbb{J} = \mathbf{1}\mathbf{1}^T$$

it follows that

$$\det(\mathbb{I} + (\alpha\mathbb{I} + \gamma A(D))^{-1}\beta\mathbb{J}) = 1 + \beta\mathbf{1}^T(\alpha\mathbb{I} + \gamma A(D))^{-1}\mathbf{1}.$$

We are working effectively over the field of real rational functions in t , therefore

$$\det(\alpha\mathbb{I} + \gamma A(D)) = \gamma^{|D|} \det\left(\frac{\alpha}{\gamma}\mathbb{I} + A(D)\right)$$

and

$$\mathbf{1}(\alpha\mathbb{I} + \gamma A(D))^{-1}\mathbf{1}^T = \alpha^{-1} \sum_{r \geq 0} \left(\frac{\gamma}{\alpha}\right)^r \langle \mathbf{1}, A^r \mathbf{1} \rangle.$$

We conclude that $\det W_{D,D}(X, t)$ is determined by

$$\alpha, \beta, \gamma, \phi(D, t)$$

and the series

$$\sum_{r \geq 0} \langle \mathbf{1}, A(D)^r \mathbf{1} \rangle t^r$$

which is the generating function for all walks in D . By Exercise 10 in Chapter 4 of [3], this generating function is determined by the characteristic polynomial of D and its complement.

Consequently we have shown that if D_1 and D_2 are induced subgraphs of X , cospectral with cospectral complements, then $X \setminus D_1$ and $X \setminus D_2$ are cospectral. Applying this to the complement of X , which is also strongly regular, we deduce that the complements of $X \setminus D_1$ and $X \setminus D_2$ are cospectral. \square

If S_1 and S_2 are independent sets of the same size in the strongly regular graph X , the previous theorem implies that $X \setminus S_1$ and $X \setminus S_2$ are cospectral. Even this special case of the theorem appears to be new.

3 Equitable Partitions

We will also be working with equitable partitions of graphs. A partition π of the vertices of X is *equitable* if for each pair of cells C_i and C_j of π there is constant $b_{i,j}$ such that each vertex in C_i has exactly $b_{i,j}$ neighbours in C_j . The *quotient graph* X/π has the cells of π as its vertices, with $b_{i,j}$ directed edges from C_i to C_j . If G is a group of automorphisms of X , then the orbits of G form an equitable partition. If X is strongly regular and $u \in V(X)$, the partition with three cells consisting of $\{u\}$, the neighbours of u , and the vertices at distance two from u is equitable.

If π is a partition, the *characteristic matrix* of π is the matrix with the characteristic vectors of the cells of π as its columns. (Thus it is a 01-matrix and each row-sum is equal to 1.) If π is an equitable partition of X with characteristic matrix R and $B := A(X/\pi)$, then

$$AR = RB.$$

There is a matrix B such that $AR = RB$ if and only if $\text{col}(R)$ is A -invariant, and this in turn holds if and only if π is equitable. If z is an eigenvector for B with eigenvalue λ , then Rz is an eigenvector for A with eigenvalue λ . This shows that each eigenvalue of B is an eigenvalue of A .

As a particularly relevant example, the symmetric square $X^{\{2\}}$ has two sorts of vertices: the pairs uv where $u \sim v$ and the pairs uv where $u \not\sim v$. If X is strongly regular with parameters $(v, k; a, c)$, then this partition is equitable with quotient matrix

$$B = \begin{pmatrix} 2a & 2k - 2a - 2 \\ 2c & 2k - 2c \end{pmatrix}.$$

If $\delta := a - c$, then the eigenvalues of this matrix are

$$k + \delta \pm \sqrt{(k - \delta)^2 - 4c},$$

and these are eigenvalues of the symmetric square. The eigenvector z of B corresponding to the positive eigenvalue is positive, and therefore Rz is a positive eigenvector of A . This implies that the positive eigenvalue is the spectral radius of the symmetric square.

We have the following relation between walks in X and X/π when π is equitable.

3.1 Lemma. *Let X be a graph with adjacency matrix A . If π is an equitable partition of X and $B := A(X/\pi)$, then the r, s -entry of B^k is equal to the number of walks of length k in X that start on a given vertex in cell C_r and finish on a vertex on C_s .*

Proof. Assume $v = |V(X)|$. Let π be an equitable partition of X with r cells and let R be the characteristic matrix of π . Then $AR = RB$ and, more generally,

$$A^k R = RB^k, \quad k \geq 0.$$

Let e_1, \dots, e_v denote the standard basis of \mathbb{R}^v and let f_1, \dots, f_r denote the standard basis of \mathbb{R}^r . Let u and v be vertices of X that form singleton cells of π , and suppose $\{v\}$ is the j -th cell of π . If $u \in V(X)$ then

$$\langle e_u, A^k R f_j \rangle$$

is the number of walks of length k in X that start at u and finish on a vertex in the j -th cell of π . On the other hand, if vertex u is in the i -th cell of π , then $R e_u = f_i$ and

$$\langle e_u, R B^k f_j \rangle = \langle f_i, B^k f_j \rangle. \quad \square$$

4 Constructing the Symmetric Square

The main result of this paper depends on the observation that we can construct the symmetric square of X in two stages.

We begin with the Cartesian product of X with itself, which has adjacency matrix

$$A \otimes \mathbb{I} + \mathbb{I} \otimes A.$$

The vertex set of the Cartesian product $X \square Y$ of X and Y is $V(X) \times V(Y)$, and $(x, y) \sim (x', y')$ if either $x = x'$ and $y \sim y'$, or $x \sim x'$ and $y = y'$. We also have

$$\text{dist}_{X \square Y}((x, y), (x', y')) = \text{dist}_X(x, x') + \text{dist}_Y(y, y').$$

We denote $X \square X$ by $X^{\square 2}$. The subgraph of $X^{\square 2}$ induced by the vertices

$$\{(i, i) : i \in V(X)\}$$

is called the *diagonal*.

The map

$$\tau : (i, j) \mapsto (j, i)$$

is an automorphism of $X^{\square 2}$. It fixes each vertex in the diagonal and partitions the remaining vertices into pairs. We will call it the *flip* automorphism of $X^{\square 2}$.

4.1 Theorem. *Let X be a graph, let D denote the diagonal of $X^{\square 2}$ and let π be the partition of $(X^{\square 2}) \setminus D$ formed by the non-trivial orbits of the flip. Then $X^{\{2\}}$ is isomorphic to $((X^{\square 2}) \setminus D)/\pi$. \square*

We make some comments on the quotienting involved. Suppose i and j are distinct vertices in X . Then $(i, j) \not\sim (j, i)$, and therefore each orbit of the flip of size two is an independent set. If $i \neq \ell$ and $(i, j) \sim (i, \ell)$, then $(i, j) \not\sim (\ell, i)$. Hence two orbits of the flip are either not joined by any edges, or else each vertex in one orbit has exactly one orbit in the second. It follows from this that $((X^{\square 2}) \setminus D)/\pi$ has no loops and no multiple edges—it is a simple graph.

Our aim now is to show that if X and Y are strongly regular graphs with the same parameters, then the graphs obtained by deleting the diagonal from $X^{\square 2}$ and $Y \square Y$ are cospectral (with cospectral complements). We will then show that the quotients modulo the flip are cospectral.

5 Deleting the Diagonal

If θ is an eigenvalue of A , let E_θ denote the orthogonal projection onto the eigenspace belonging to θ . Then if $r \geq 0$, we have the spectral decomposition:

$$A^r = \sum_{\theta} \theta^r E_\theta.$$

from which we have

$$W(X, t) = \sum_{\theta} (1 - t\theta)^{-1} E_\theta.$$

Since

$$A \otimes \mathbb{I} + \mathbb{I} \otimes A = \sum_{\theta, \tau} (\theta + \tau) E_{\theta} \otimes E_{\tau},$$

we see that

$$W(X^{\square 2}, t) = \sum_{\theta, \tau} (1 - t(\theta + \tau))^{-1} E_{\theta} \otimes E_{\tau}.$$

If M and N are $m \times n$ matrices, their *Schur product* (also called Hadamard product) $M \circ N$ is the $m \times n$ matrix given by

$$(M \circ N)_{i,j} = M_{i,j} N_{i,j}.$$

5.1 Theorem. *If D denotes the diagonal of $X^{\square 2}$ and $A(X)$ has the spectral decomposition $\sum_{\theta} \theta E_{\theta}$, then*

$$W_{D,D}(X^{\square 2}, t) = \sum_{\theta, \tau} (1 - t(\theta + \tau))^{-1} E_{\theta} \circ E_{\tau}.$$

Proof. It is enough to note that

$$(E_{\theta} \otimes E_{\tau})_{D,D} = E_{\theta} \circ E_{\tau}. \quad \square$$

The linear span of the principal idempotents of the adjacency matrix of a strongly regular graph is equal to the span of \mathbb{I} , $A(X)$ and \mathbb{J} , and is therefore closed under the Schur product. Hence $E_{\theta} \circ E_{\tau}$ is a linear combination of principal idempotents. The coefficients in this linear expansion are known as the *Krein parameters* of the strongly regular graph, and are determined by the parameters of the graph. Therefore the eigenvalues of $W_{D,D}(X^{\square 2}, t)$ are determined by the parameters of X , and so $\det(W_{D,D}(X^{\square 2}, t))$ is determined by the parameters of X .

5.2 Lemma. *If X is a strongly regular graph and D is the diagonal of $X^{\square 2}$, then the spectrum of $X^{\square 2} \setminus D$ is determined by the spectrum of X .* \square

6 Flipping Quotients

We use Y to denote the quotient of $X^{\square 2}$ by the flip. By Lemma 3.1 we have the following.

6.1 Lemma. *If Y denotes the quotient of $X^{\square 2}$ by the flip and D denotes both the diagonal of $X^{\square 2}$ and the image of D in Y , then*

$$\frac{\phi(Y \setminus D, t)}{\phi(Y, t)} = \frac{\phi(X^{\square 2} \setminus D, t)}{\phi(X^{\square 2}, t)}.$$

We now show that, for any graph X , the spectrum of Y is determined by the spectrum of X . Given the above lemma it follows immediately that if X is strongly regular, then the spectrum of $X^{\{2\}}$ is determined by the spectrum of X .

Let X_1 and X_2 be two cospectral graphs on v vertices with adjacency matrices A_1 and A_2 . Let L be an orthogonal matrix such that

$$L^T A_1 L = A_2.$$

Let \mathbb{F} be the permutation matrix that represents the flip on $\mathbb{R}^v \otimes \mathbb{R}^v$. So \mathbb{F} maps $x \otimes y$ to $y \otimes x$, for all x and y in \mathbb{R}^v . Let R be the normalized characteristic matrix of the orbit partition of the flip— R is obtained from the characteristic matrix of the orbit partition by normalizing each column. We have

$$R^T R = \mathbb{I}, \quad R R^T = \frac{1}{2}(\mathbb{I} + \mathbb{F}).$$

Let $A_i^{\square 2}$ denote the adjacency matrix of $X_i^{\square 2}$. Then there are matrices C_i such that

$$A_i^{\square 2} R = R C_i$$

We prove that C_1 and C_2 are cospectral.

We have

$$C_2 = R^T A_2^{\square 2} R = R^T (L \otimes L)^T A_1^{\square 2} (L \otimes L) R$$

whence

$$R C_2 R^T = R R^T (L \otimes L)^T A_1^{\square 2} (L \otimes L) R R^T.$$

Because $L \otimes L$ and \mathbb{F} commute, so do $L \otimes L$ and $R R^T$. So

$$R C_2 R^T = (L \otimes L)^T R R^T A_1^{\square 2} R R^T (L \otimes L) = (L \otimes L)^T R C_1 R^T (L \otimes L)$$

and hence

$$C_2 = R^T (L \otimes L)^T R C_1 R^T (L \otimes L) R.$$

Since

$$\begin{aligned} R^T (L \otimes L)^T R R^T (L \otimes L) R &= R^T (L \otimes L)^T (L \otimes L) R R^T R \\ &= R^T R R^T R \\ &= \mathbb{I}, \end{aligned}$$

we conclude that C_1 and C_2 are similar matrices.

Note that it is possible to express the spectrum of Y in terms of the spectrum of X . If π is equitable and $B = A(X/\pi)$ and θ is an eigenvalue of B , then

$$\dim(\ker(B - \theta \mathbb{I})) = \dim(\text{col}(R) \cap \ker(A - \theta \mathbb{I})).$$

Suppose z_1, \dots, z_n is an orthonormal basis for \mathbb{R}^n consisting of eigenvectors of X . Then the products $z_i \otimes z_j$ form an orthonormal basis for \mathbb{R}^{n^2} consisting of

eigenvectors of $X^{\square 2}$. If $i \neq j$ then the span of z_i and z_j is equal to the span of the symmetric and antisymmetric combinations

$$(z_i \otimes z_j) + (z_j \otimes z_i), \quad (z_i \otimes z_j) - (z_j \otimes z_i)$$

These two vectors are orthogonal and the first is constant on the orbit partition of the flip, while the second sums to zero on each orbit. If $z^T A = \theta z$ then $z^T R B = \theta z^T R$. So if θ has multiplicity ℓ as an eigenvalue of X , the vectors

$$(z_i \otimes z_j) + (z_j \otimes z_i), \quad z_i \otimes z_i,$$

where $z_i \in \ker(A - \theta \mathbb{I})$, give rise to a subspace of eigenvectors of Y with eigenvalue 2θ and dimension $\binom{\ell+1}{2}$. If θ has multiplicity ℓ and τ has multiplicity m , then we obtain a subspace of eigenvectors of the quotient with dimension ℓm . By adding up the dimensions of these subspaces, we find that the images of the given vectors provide a basis consisting of eigenvectors of Y . It follows that the multiplicities of the eigenvalues of Y are determined by the eigenvalues of X and their multiplicities. (If X has exactly r distinct eigenvalues, then $X^{\square 2}$ has at most $\binom{r+1}{2}$; if $X^{\square 2}$ has fewer eigenvalues, then the procedure just described will give the multiplicities of the eigenvalues of Y , but does not lead to a simple formula.)

7 More Cospectral

We have seen that if X and Y are strongly regular graphs with the same parameters, then their symmetric squares are cospectral. Here we extend this.

7.1 Lemma. *If X and Y are strongly regular graphs with the same parameters, then the complements of their symmetric squares are cospectral.*

Proof. \imath From Exercise 22 in Chapter 2 of [3], we have

$$\phi(\overline{X}, t+1) = (-1)^v \phi(X, t) (1 - \mathbf{1}^T (tI + A)^{-1} \mathbf{1}).$$

\imath From this it follows that cospectral graphs X and Y have \imath cospectral complements if and only if the generating function for all walks in X is equal to the corresponding generating function for Y .

Assume X is strongly regular, let A denote the adjacency matrix of $X^{\{2\}}$, let π be the partition of the vertices of $X^{\{2\}}$ by valency and let the characteristic matrix R and quotient matrix B be defined as in Section 3. Then $AR = RB$ and so, for if $\ell \geq 0$,

$$A^\ell R = RB^\ell.$$

Since the columns of R sum to $\mathbf{1}$,

$$\mathbf{1}^T A^\ell \mathbf{1}^T = \mathbf{1}^T A^\ell R \mathbf{1} = \mathbf{1}^T R B^\ell \mathbf{1}.$$

We have

$$\mathbf{1}^T R = (vk/2, v(v-1-k)/2)$$

and therefore the entries of $R^T B^\ell$ are determined by ℓ and the parameters of X . Hence the generating function for all walk in $X^{\{2\}}$ is determined by the parameters of the strongly regular graph X , and the result follows. \square

8 Variations

The *direct product* $X \times Y$ of graphs X and Y has vertex set equal to $V(X) \times V(Y)$, and $(u, v) \sim (x, y)$ if and only if $u \sim x$ and $v \sim y$. We have

$$A(X \times Y) = A(X) \otimes A(Y).$$

The flip map

$$(x, y) \mapsto (y, x)$$

is again an automorphism of $X \times X$ that fixes the diagonal. We can obtain an analog of the symmetric product by deleting the diagonal and then quotienting over the flip. A slightly modified version of the argument in this paper shows that if X is strongly regular, then the spectrum of this analog is determined by the spectrum of X . The key step is to verify the following analog of Theorem 5.1:

$$W_{D,D}(X^{\otimes 2}, t) = \sum_{\theta, \tau} (1 - t\theta\tau)^{-1} E_\theta \circ E_\tau.$$

For a second analog, we turn to the graph obtained from the Cartesian power $X^{\square k}$ by deleting the diagonal and the quotienting over the orbits of the automorphism that sends each k -tuple to its right cyclic shift. Again our argument shows that if X is strongly regular, the spectrum of this analog is determined by X . Thus there is more than one candidate for the ‘‘symmetric cube’’ of a graph, but the spectrum of the one just described is a less useful graph invariant than the spectrum of the symmetric cube defined in Section 1.

9 Symmetric Squares of General Graphs

In this section we take a closer look at the purely algebraic properties of the symmetric powers, and of the symmetric square in particular. We start by giving a purely algebraic definition.

Let $P^{(k)}$ be the 0/1-matrix with $\binom{v}{k}$ rows, labelled by the k -tuples (i, j, \dots, l) with $1 \leq i < j < \dots < l \leq v$, and v^k columns, labelled by the k -tuples $[i', j', \dots, l']$ with $1 \leq i', j', \dots, l' \leq v$, such that the elements $P_{(i,j,\dots,l),[i',j',\dots,l']}^{(k)}$ are 1 iff (i, j, \dots, l) is a permutation of $[i', j', \dots, l']$. Then

9.1 Lemma. *The adjacency matrix $A^{\{k\}}(X)$ of $X^{\{k\}}$ is*

$$A^{\{k\}}(X) = \frac{1}{(k-1)!} P^{(k)} (A(X) \otimes \mathbb{I}_v^{\otimes k-1}) P^{(k)*}$$

We focus on the symmetric square, and more generally on the properties of the linear map

$$\Omega : G \mapsto \Omega(G) \equiv G^{\{2\}} = P^{(2)}(G \otimes \mathbb{I})P^{(2)*}.$$

Henceforth, we will write P instead of $P^{(2)}$.

Because Ω is the composition of the two completely positive maps [6] $A \mapsto A \otimes \mathbb{I}$ and $A \mapsto BAB^*$, Ω is completely positive itself. In particular, Ω preserves positive semi-definiteness. One easily checks

$$PP^* = 2\mathbb{I}_{\binom{d}{2}} \quad (1)$$

$$P^*P = \sum_{i,j=1}^d (E_{ii} \otimes E_{jj} + E_{ij} \otimes E_{ji}) - 2 \sum_{i=1}^v E_{ii} \otimes E_{ii}, \quad (2)$$

where $\{E_{ij}\}$ is the standard matrix basis.

The spectrum of a general Hermitian matrix and the spectrum of its symmetric square have the same average value. When G is an adjacency matrix this obviously has no import, because adjacency matrices are traceless. However, in certain quantum mechanical contexts the map Ω is applied to Hamiltonians which are not traceless.

9.2 Theorem. *For G a $v \times v$ Hermitian matrix,*

$$\mathrm{Tr}[G]/v = \mathrm{Tr}[G^{\{2\}}]/\binom{v}{2}.$$

Proof. The partial trace of P^*P over the second tensor factor, defined as $\mathrm{Tr}[(X \otimes \mathbb{I})A] = \mathrm{Tr}[X \mathrm{Tr}_2[A]]$, yields

$$\begin{aligned} \mathrm{Tr}_2[P^*P] &= \sum_{i,j=1}^v (E_{ii} \mathrm{Tr}[E_{jj}] + E_{ij} \mathrm{Tr}[E_{ji}]) - 2 \sum_{i=1}^v E_{ii} \mathrm{Tr}[E_{ii}] \\ &= \sum_{i,j=1}^v (E_{ii} + E_{ij}\delta_{ij}) - 2 \sum_{i=1}^v E_{ii} \\ &= (v-1)\mathbb{I}_v. \end{aligned}$$

Therefore,

$$\begin{aligned} \mathrm{Tr}[\Omega(G)] &= \mathrm{Tr}[P^*P(G \otimes \mathbb{I})] \\ &= \mathrm{Tr}[G \mathrm{Tr}_2[P^*P]] \\ &= (v-1) \mathrm{Tr}[G]. \end{aligned}$$

Dividing by $v(v-1)$ yields the statement of the Theorem. \square

9.1 Comparison between the spectrum of a matrix and the spectrum of its symmetric square

For a Hermitian matrix A , we denote by $\lambda_k^\downarrow(A)$ its k -th largest eigenvalue, counting multiplicities. Likewise, $\lambda_k^\uparrow(A)$ is its k -th smallest eigenvalue.

We prove the following:

9.3 Theorem. *For any non-negative positive semi-definite $v \times v$ matrix G , the following relation holds, for $1 \leq m \leq v$:*

$$\lambda_m^\downarrow(G) \leq \lambda_m^\downarrow(\Omega(G)).$$

Proof. We refer to [4] or [5] for the basic matrix analytical concepts and theorems.

say it at all :-) Focusing on a particular value of m , $1 \leq m \leq v$, we need to show

$$\lambda_m^\downarrow(G) \leq \lambda_m^\downarrow(P(G \otimes \mathbb{I})P^*),$$

for all $G \geq 0$, or, equivalently,

$$\lambda_m^\downarrow(P(G \otimes \mathbb{I})P^*) \geq 1, \tag{3}$$

for all $G \geq 0$ with $\lambda_m^\downarrow(G) = 1$.

First note that one needs to prove this only for G a partial isometry of rank m . Indeed, for every $G \geq 0$ with $\lambda_m^\downarrow(G) = 1$, there exists a partial isometry B of rank m such that $G \geq B$. As noted above, Ω is a completely positive map, hence $\Omega(G) \geq \Omega(B)$. By Weyl monotonicity we then have $\lambda_m^\downarrow(\Omega(G)) \geq \lambda_m^\downarrow(\Omega(B))$. Thus (3) follows for G if it holds for B .

Let us write B as $B = Q^*Q$, with $Q \in M_{m,v}(\mathbb{C})$ and $QQ^* = \mathbb{I}_m$. Let q_j be the j -th column of Q . Thus the q_j are v k -dimensional vectors and

$$\sum_{j=1}^v q_j q_j^* = \mathbb{I}_m.$$

The matrix $P(Q^*Q \otimes \mathbb{I})P^*$ has the same non-zero eigenvalues as

$$(Q \otimes \mathbb{I})P^*P(Q^* \otimes \mathbb{I}).$$

Using the explicit form (2), a short calculation shows that

$$\lambda_m^\downarrow(\Omega(Q^*Q)) = \lambda_m^\downarrow(\mathbb{I} + A) = 1 + \lambda_m^\downarrow(A),$$

where A is a $v \times v$ block matrix with blocks $A_{i,j}$ of size $m \times m$ given by

$$A_{i,j} = (1 - 2\delta_{ij})q_j q_i^*.$$

We have

$$\sum_{i=1}^v A_{i,i} = -\mathbb{I}_m.$$

We have to show that $\lambda_m^\perp(A) \geq 0$. To that purpose, consider the principal submatrix A' of A consisting of the 2×2 upper left blocks:

$$A' = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = \begin{pmatrix} -q_1 q_1^* & q_2 q_1^* \\ q_1 q_2^* & -q_2 q_2^* \end{pmatrix}.$$

If we can prove that $\lambda_m^\perp(A') \geq 0$, this implies $\lambda_m^\perp(A) \geq 0$ via eigenvalue interlacing.

When $m = 1$, the q_i are scalars, and direct calculation shows that $\lambda_1^\perp(A') = 0$.

For $m > 1$, consider a (non-orthogonal) basis of \mathbb{C}^d in which q_1 and q_2 are the first basis vectors. Let S be the transformation from this new basis to the standard basis. Under the *-congruence governed by S , A' is transformed to

$$SA'S^* = \left(\begin{array}{cccc|cccc} -1 & & & & 0 & & & \\ & 0 & & & 1 & & & \\ & & \ddots & & \vdots & & & \\ & & & 0 & 0 & & & \\ \hline & 0 & 1 & \dots & 0 & 0 & & \\ & & & & & -1 & & \\ & & & & & & \ddots & \\ & & & & & & & 0 \end{array} \right).$$

This matrix has eigenvalues -1 , with multiplicity 3, 0 , with multiplicity $2m - 4$, and 1 , with multiplicity 1. By Sylvester's Law of Inertia, a *-congruence does not change the sign of the eigenvalues. Thus A' has $2m - 3$ non-negative eigenvalues as well. Hence, for $m > 2$, $\lambda_m^\perp(A') \geq 0$.

To cover the remaining case of $m = 2$, we first perform a specific *-congruence on A directly. For $m = 2$ there are only 2 independent vectors q_j . Let S_1 be the transformation that brings q_1 to $(1, 0)$, and q_2 to $(0, 1)$. Let q_3 be brought to (x, y) . We can assume without loss of generality that $q_3 \neq q_2$, so that $x \neq 0$. The 3×3 upper left blocks of $S_1 A S_1^*$ will thus be

$$\left(\begin{array}{cc|cc|cc} -1 & 0 & 0 & 0 & x & 0 \\ 0 & 0 & 1 & 0 & y & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & x \\ 0 & 0 & 0 & -1 & 0 & y \\ \hline x^* & y^* & 0 & 0 & -|x|^2 & -xy^* \\ 0 & 0 & x^* & y^* & -x^*y & -|y|^2 \end{array} \right).$$

One further *-congruence $S_2 = \mathbb{I} + E_{1,5}/x^*$ brings this to $S_2 S_1 A S_1^* S_2^*$, with 3×3 upper left blocks

$$\left(\begin{array}{cc|cc|cc} 0 & (y/x)^* & 0 & 0 & 0 & -x(y/x)^* \\ y/x & 0 & 1 & 0 & y & 0 \\ \hline 0 & 1 & 0 & 0 & 0 & x \\ 0 & 0 & 0 & -1 & 0 & y \\ \hline 0 & y^* & 0 & 0 & -|x|^2 & -xy^* \\ -x^*y/x & 0 & x^* & y^* & -x^*y & -|y|^2 \end{array} \right).$$

The upper left 3×3 principal submatrix is of the form

$$\begin{pmatrix} 0 & z^* & 0 \\ z & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix},$$

which has eigenvalues 0 and $\pm\sqrt{1+|z|^2}$, i.e. it has two non-negative eigenvalues. By the interlacing theorem, $S_2 S_1 A S_1^* S_2^*$ must then also have at least two non-negative eigenvalues, and by Sylvester's Law of Inertia, A itself too. \square

Because of the restriction to positive semi-definite matrices, Theorem 9.3 can only be applied directly to graph invariants formed from, say, the spectrum of the Laplacian matrix $L(X)$ of the graph under the map Ω . The following Corollary extends Theorem 9.3 to Hermitian G that are not necessarily positive semi-definite, and can therefore be applied to adjacency matrices proper:

9.4 Corollary. *For any Hermitian $v \times v$ matrix G ,*

$$(\lambda_k^\downarrow(G) + \lambda_v^\downarrow(G))/2 \leq \lambda_k^\downarrow(G^{\{2\}}/2) \quad (4)$$

$$(\lambda_k^\uparrow(G) + \lambda_v^\uparrow(G))/2 \geq \lambda_k^\uparrow(G^{\{2\}}/2). \quad (5)$$

Proof. Let $\alpha = \lambda_v^\downarrow(G)$, then $G' := G + \alpha\mathbb{I} \geq 0$. Applying Theorem 9.3 to G' gives

$$\lambda_m^\downarrow(G + \alpha\mathbb{I}) \leq \lambda_m^\downarrow(\Omega(G + \alpha\mathbb{I})).$$

Noting that $\Omega(\mathbb{I}) = PP^*$, which has the same non-zero eigenvalues as $P^*P = 2\mathbb{I}_{\binom{v}{2}}$, yields

$$\lambda_m^\downarrow(G) + \alpha \leq \lambda_m^\downarrow(\Omega(G)) + 2\alpha,$$

and the first inequality of the Corollary follows. The second inequality follows by applying the first one to $-G$. \square

Very likely, the bound of Theorem 9.3 (and the Corollary) can be sharpened. However, it cannot be sharpened by more than a factor of 2. This can be seen by taking as G a rank- k partial isometry, for which $\lambda_k^\downarrow(G) = 1$, and noting that by inequality (5) (with $k = v$), $G \leq \mathbb{I}$ implies $G^{\{2\}} \leq 2\mathbb{I}$. Hence, for this particular G , $\lambda_k^\downarrow(G^{\{2\}}) \leq 2\lambda_k^\downarrow(G)$, which would contradict a sharpening of Theorem 9.3 by a factor of more than 2.

9.2 On the nature of $P^{(k)}$

In this section we consider the $P^{(k)}$ appearing in the definition of the symmetric power, and compare it to the two related operators P_\vee and P_\wedge , which are projections from the k -fold tensor power of \mathbb{C}^v to its totally symmetric and totally antisymmetric subspace, respectively ([5], Section I.5). Formally, P_\vee and P_\wedge are defined as those linear operators that map a tensor product of k vectors

from \mathbb{C}^d to their symmetric and antisymmetric tensor product, respectively,

$$\begin{aligned} P_V(x_1 \otimes \cdots \otimes x_k) &= (k!)^{-1} \sum_{\sigma} x_{\sigma(1)} \otimes \cdots \otimes x_{\sigma(k)} \\ P_{\wedge}(x_1 \otimes \cdots \otimes x_k) &= (k!)^{-1} \sum_{\sigma} \epsilon_{\sigma} x_{\sigma(1)} \otimes \cdots \otimes x_{\sigma(k)}, \end{aligned}$$

where the sum is over all permutations σ of k objects, and ϵ_{σ} is the signature of σ . The operator $P^{(k)}$ is similar to P_V in that tensor products that differ in the ordering of factors only are mapped to one and the same vector; it is similar to P_{\wedge} in that it maps to a space of the same dimension as the totally antisymmetric subspace and maps tensor products containing identical factors to 0.

To describe this in a more formal manner, consider the basis of the totally antisymmetric subspace consisting of the vectors

$$\begin{aligned} e_{(i,j,\dots,l)} &= e_i \wedge e_j \wedge \cdots \wedge e_l \\ &:= (k!)^{-1/2} \sum_{\sigma} \epsilon_{\sigma} e_{\sigma(i)} \otimes e_{\sigma(j)} \otimes \cdots \otimes e_{\sigma(l)}, \end{aligned}$$

labelled by the k -tuples $(i, j \dots l)$ with $1 \leq i < j < \dots < l \leq d$. Then $P^{(k)}$ maps the vector $e_{i'} \otimes e_{j'} \otimes \cdots \otimes e_{l'}$, where $[i', j', \dots, l']$ is a k -tuple with $1 \leq i', j', \dots, l' \leq d$, to the vector $e_{(i,j,\dots,l)}$, with k -tuple $(i, j \dots l)$ equal to the k -tuple $[i', j', \dots, l']$ sorted in ascending order, provided $[i', j', \dots, l']$ does not contain equal indices, and to 0 otherwise. The difference between $P^{(k)}$ and P_{\wedge} is the absence of the sign ϵ_{σ} of the permutation that realises the sorting. Note, for $k = 2$,

$$\begin{aligned} P_{\wedge}^* P_{\wedge} &= (\mathbb{I} - \mathbb{F})/2 \\ P_V^* P_V &= (\mathbb{I} + \mathbb{F})/2, \end{aligned}$$

where \mathbb{F} is the flip operator defined in section 6.

In the following we look at the map $G \mapsto G^{\vee} := P_V(G \otimes \mathbb{I}^{\otimes k-1})P_V^*$. Because of the symmetry of P_V ,

$$\begin{aligned} G^{\vee} &= \frac{1}{k} P_V(G \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I} + \mathbb{I} \otimes G \otimes \mathbb{I} \otimes \cdots \otimes \mathbb{I} + \cdots + \mathbb{I} \otimes \mathbb{I} \otimes \cdots \otimes A)P_V^* \\ &= \frac{1}{k} \left. \frac{\partial}{\partial t} \right|_{t=0} P_V(\mathbb{I} + tG)^{\otimes k} P_V^*. \end{aligned}$$

The expression $P_V(\mathbb{I} + tG)^{\otimes k} P_V^*$ is nothing but the totally symmetric irreducible representation of $\mathbb{I} + tG$ on k copies of \mathbb{C}^v . It is well-known from representation theory that the eigenvalues of an irreducible representation of a matrix A depend only on the eigenvalues of A itself. Therefore, we find that the spectrum of $P_V(G \otimes \mathbb{I}^{\otimes k-1})P_V^*$ depends on the spectrum of G only. In other words, if G_1 and G_2 are cospectral, then so are G_1^{\vee} and G_2^{\vee} . A similar reasoning applies when using P_{\wedge} instead of P_V .

It is therefore remarkable that $\Omega(G_1)$ and $\Omega(G_2)$ need not be cospectral even if G_1 and G_2 are, given that $P^{(k)}$ is a combination of P_\vee and P_\wedge . This is one of the underlying reasons why we chose to study Ω in the context of the graph isomorphism, the other reason being its physical relevance (as discussed in the appendix).

10 Computational Results

Strongly regular graphs, and to a somewhat lesser extent walk-regular graphs, satisfy very strong combinatorial and algebraic regularity conditions, and it might be hoped that this was closely related to the occurrence of cospectral symmetric squares. Unfortunately our computational results show that this is not the case, and that in fact graphs with cospectral symmetric squares occur in relative abundance. Nevertheless, the examples that we have found do have some interesting algebraic properties that may go some way towards explaining when symmetric squares are cospectral.

We have checked all graphs on up to 10 vertices without finding any pairs of graphs with cospectral symmetric squares, and currently the smallest pairs that we know have 16 vertices. There are only two pairs of cospectral strongly regular graphs on 16 vertices, but using a variety of heuristic search techniques, we have constructed more than 30000 further graphs on 16 vertices that have a partner with a cospectral symmetric square. These heuristics involve first using direct searches of catalogues of strongly regular graphs, vertex-transitive graphs and regular graphs to generate an initial collection of example pairs. Then we construct large numbers of closely-related graphs by making a variety of minor modifications to these initial graphs, such as exchanging pairs of edges, removing one or more vertices, removing one or more edges, or adding or deleting one-factors. These graphs are then searched for further non-isomorphic pairs of graphs with cospectral squares, and any new examples added to the growing list. By repeatedly applying these techniques, we can obtain pairs of graphs that are seemingly very different to the initial examples, but that have cospectral symmetric squares.

Using these techniques, we have found it easy to construct many pairs of graphs on 16 or more vertices cospectral squares. We have put considerable effort in constructing as many graphs as possible on 16 vertices, but due to the techniques involved, we do not speculate as to whether these 30000+ graphs might comprise most of, or almost none of, the full collection of examples on 16 vertices. All our efforts to construct examples on fewer than 16 vertices have failed.

The examples that we have constructed do not show any strong graph-theoretical structure, most of them are not regular, and there are many examples with trivial automorphism group. However the pairs of graphs with cospectral symmetric squares do exhibit interesting algebraic behaviour that is not *a priori* necessary in order to have cospectral symmetric squares. In particular, for all of the known pairs of graphs $\{X, Y\}$ such that $X^{\{2\}}$ and $Y^{\{2\}}$ are cospectral,

the following properties also hold:

- (a) X and Y are cospectral, and \overline{X} and \overline{Y} are cospectral,
- (b) The symmetric squares of \overline{X} and \overline{Y} are cospectral,
- (c) The complements of the symmetric squares of X and Y are cospectral
- (d) The multisets $\{\varphi(X \setminus i) : i \in V(X)\}$ and $\{\varphi(Y \setminus i) : i \in V(Y)\}$ are equal,
- (e) The multisets $\{\varphi(X \setminus ij) : i, j \in V(X)\}$ and $\{\varphi(Y \setminus ij) : i, j \in V(Y)\}$ are equal.

If X and Y are strongly regular graphs with the same parameters, then all of these five properties hold (the third one requires a non-trivial argument), but in general we do not know whether or not these are necessary conditions for X and Y to have cospectral symmetric squares.

There are 32548 strongly regular graphs with parameters $(36, 15, 6, 6)$ each of whose symmetric cubes has 7140 vertices. Performing exact calculations of characteristic polynomials on matrices of this size requires highly specialized software, and the only such software of which we are aware is that being developed by the LinBox team (see www.linalg.org). Proving that two graphs are *not* cospectral is easier in that if there is some $\alpha \in GF(p)$ (where p is a large prime) such that $\det(A_1 + \alpha I) \neq \det(A_2 + \alpha I) \pmod{p}$ then A_1 and A_2 are definitely not cospectral. We would like to thank the LinBox team, particularly Jean-Guillaume Dumas, Clément Pernet and David Saunders for planning and performing computations using this technique that demonstrated that none of the SRGs on 35 or 36 vertices have cospectral symmetric cubes.

11 Acknowledgements

This work was supported by The Leverhulme Trust grant F/07 058/U, and is part of the QIP-IRC (www.qipirc.org) supported by EPSRC (GR/S82176/0). Godsil's work is supported by NSERC.

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12 Appendix: Quantum Hamiltonians and Symmetric Powers

Consider a generic set of n distinguishable two-dimensional quantum systems (qubits). Letting $|0\rangle, |1\rangle$ be a basis for \mathbb{C}^2 , and defining raising and lowering operators for qubit i :

$$S_i^+ = |1\rangle\langle 0|, S_i^- = |0\rangle\langle 1|,$$

a commonly encountered interaction Hamiltonian for the systems is of exchange form:

$$H_{\text{int}} = \sum_{ij} g_{ij} (S_i^+ S_j^- + S_i^- S_j^+)$$

where g_{ij} is the interaction energy between qubits i and j . For instance, the systems could be two-level atoms in a molecule, interacting via a dipole-dipole interaction; spins on a lattice interacting via an “ XY ” spin-exchange interaction; or hard-core bosons hopping around some lattice structure (Bose-Hubbard model).

In certain situations the relevant physics lies only in the properties of this interaction Hamiltonian. For instance, for the two-level atoms the free Hamiltonian is trivial and can be ignored by going to the ‘interaction picture’. In the limit of hard-core bosons in a Hubbard model, the interaction energy dominates the single-site energy, and double occupancy of a site is forbidden. In such scenarios, if it is also approximately true that the interaction strength is the same regardless of the pair of systems under consideration (no distance dependent interactions for instance) then we can take $g_{ij} = 1, 0$ according to whether qubits i and j are coupled or not. This simplified interaction Hamiltonian is then

$$H_{\text{int}} = \bigoplus_{k=1}^n X^{\{k\}}$$

i.e., a direct sum of the symmetric powers of the underlying graph X , whose adjacency matrix is g_{ij} .

There are two main types of graphs that generally come under consideration in physics, neither of which are particularly interesting from the graph theoretic point of view: (i) Small, (generally planar) graphs corresponding to molecular systems. (Does the excitation spectrum of a molecule determine its structure?) (ii) Large ‘local’ graphs in $\mathbb{R}^{1,2,3}$ corresponding to nearest neighbour interactions - in general some sort of standard lattice structure. In the latter case the interesting physical properties (phase transitions, super conductivity, etc.) generally appear for a number of excitations $k \approx n/2$.

To understand the strength of graph invariants formed from such Hamiltonians, and the complexity of dealing with such Hamiltonians in physics, the following observation (discussed formally in section 9.2) is useful: The subspace of the full Hilbert space in which the k 'th excitation block of the Hamiltonian lives is one of both bosonic and fermionic nature. Although the Hamiltonian is strictly speaking bosonic, fermionic features arise due to it not being possible for two excitations to reside in the same qubit. Thus, the bosons, instead of living in the $\binom{n+k-1}{k}$ dimensional symmetric tensor power subspace $\vee^k \mathcal{H}$, rather live in an “unsigned” version of the antisymmetric tensor power space $\wedge^k \mathcal{H}$. (“Unsigned” refers to the fact that the antisymmetry is not present). If, instead of living in such a hybrid “Fermi-Bose” subspace of Hilbert space, the excitations were to live in these more standard subspaces, it is easy to see that their spectra would essentially be equivalent to that of the single particle spectra (the standard graph spectrum).

Finally, it should be noted that an efficient quantum circuit simulating evolution under H_{int} is guaranteed to exist by various standard results in the theory of quantum computation. This opens up the interesting possibility that graph invariants based on symmetric k -th powers of a graph for $k = O(v)$ are quantum computationally tractable, whereas classical tractability would seem to require that $k = O(1)$.