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QUANTUM MORPHISMS

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1 Homomorphisms

1.1 Graph Homomorphisms

A graph homomorphism ψ from X to Y is a map from $V(X)$ to $V(Y)$ such that if a and b are adjacent vertices in X, then $\psi(a)$ and $\psi(b)$ are adjacent in Y. We see at once that a proper m-colouring of a graph X is a homomorphism from X to K_m, and any graph isomorphism is also a graph homomorphism. We assume that our graphs do not have loops, which implies that for each vertex u in Y, the preimage

$$\psi^{-1}(u) := \{a : \psi(a) = u\}$$

is a coclique. We refer to $\psi^{-1}(u)$ as the *fibre* of ψ at u.

The fibres of ψ form a partition of the vertices of X and[1] we represent this partition by its characteristic matrix $F(\psi)$. This is the $|V(X)| \times |V(Y)|$ matrix where the column indexed by u in $V(Y)$ is the characteristic vector of $\psi^{-1}(u)$. This F is a 01-matrix whose column sum to $\mathbf{1}$, hence its columns are orthogonal (equivalently $F^T F$ is diagonal).

[1] as is our custom

1.1.1 Lemma. *Assume F is the characteristic matrix of a partition of $V(X)$, with cells indexed by $V(Y)$. Then F is the characteristic matrix of a homomorphism if and only if whenever a, b are adjacent vertices in X and u, v are distinct non-adjacent vertices in Y, we have $F_{a,u}F_{b,v} = 0$.* □

The virtue of this lemma does not lie in any insight it provides about graph homomorphisms, but in the fact that it will allow us to establish the connections between the classical graph homomorphisms we have just defined and the quantum graph homomorphisms.[2]

[2] yet to come

1.2 The Category of Graph Homomorphisms

You may have a lot of reading to do, we will take much for granted. A *category* consists of objects and arrows. Each arrow has a domain and a codomain, and in many cases it corresponds to a function. We write things like $f : X \to Y$ to denote that f is an arrow with domain X and codomain Y. Arrows compose associatively, and for each object X there is a unique identity arrow (wth domain and codomain X). We will use $f \circ g$ to denote the composition of f and g.

Two examples. If $\mathscr{P}$ is a partially ordered set we may form a category with the elements of $\mathscr{P}$ as objects and with $a \to b$ if $a \le b$. Here the arrows are not functions. (We are labouring over this point, because quantum homomorphisms are not functions.) Our second example is the category $\mathscr{G}$ with loopless graphs as objects and graph homomorphisms as arrows.

Suppose $\mathscr{C}$ is a category. We define products, in two ways. The *product* (if it exists) of X and Y is an object denoted $X \times Y$ equipped with arrows

$$\pi_X : X \times Y \to X, \quad \pi_Y : X \times Y \to Y$$

with the following property: if there is an object Z and arrows

$$f : Z \to X, \quad g : Z \to Y$$

then there is a unique arrow $h : Z \to X \times Y$ such that

$$f = h \circ \pi_X, \quad g = h \circ \pi_Y$$

This leads to two exercises. Prove that in $\mathscr{P}$, the product of a and b is the least upper bound of a and b (if it exists). In $\mathscr{G}$, the product of X and Y is the diret product $X \times Y$.

Now we work towards a second definition of products. A *terminal object* in a category is an object, Z say, such that for each object X in $\mathscr{C}$, there is a unique homomorphism from X to Z. The identity group is a terminal object in the category of groups and group homomorphisms. The dual to a terminal object is an *initial object*. The integers are an initial object in the category of rings. Any two terminal objects are isomorphic. (Ditto for initial.)

We construct a new category. Let X and Y be graphs. The objects of our new category are triples (F, f_X, f_Y) where f_X and f_Y are homomorphisms from F to X and Y respectively. The arrows from (F, f_X, f_Y) to (G, g_X, g_Y) are the graph homomorphisms φ from F to G such that

$$g_X \circ \varphi = f_X, \quad g_Y \circ \varphi = f_Y.$$

The triple $(X \times Y, \pi_X, \pi_Y)$ is a terminal object in this category.

1.3 Exponentials

An example. If A and S are sets, we use A^S to denote the set of functions from S to A. For three sets A, B, C we have the identity

$$A^{B \times C} = (A^B)^C$$

Taking cardinalities, we deduce the exponential law for non-negative integers:

$$a^{(bc)} = (a^b)^c.$$

For graphs X and Y we define a new graph X^Y such that, for any graphs Z, the homomorphisms from Z to X^Y correspond to the homomorphisms from $Y \times Z$ to X. The key is to consider the case $Z = K_2$. The homomorphisms from K_2 to a graph X may be identified with the edges of X, so the edges of X^Y must correspond to homomorphisms from $Y \times K_2$ to X. We describe these homomorphisms in detail.

Assume $V(K_2) = \{1,2\}$; the vertices of $Y \times K_2$ are then pairs $(u,1)$ and $(v,2)$ for vertices u, v of Y. If $f : Y \times K_2 \to X$ is a homomorphism, define f_i (for $i = 0,1$) to be the restriction of f to the set $\{(u,i) : u \in V(Y)\}$. Here f_0 and f_1 are maps from $V(Y)$ to $V(X)$, our problem is to decide which pairs of maps $V(Y)$ to $V(X)$ arise as restrictions of a homomorphism. This is not difficult, f_0 and f_1 determine a homomorphism if whenever u and v are adjacent in Y, the vertices $f_0(u)$ and $f_1(v)$ are adjacent in X. In this case we say that the functions f_0 and f_1 are compatible on Y.

The above discussion is informal. We now define the graph X^Y. Its vertices are the functions from $V(Y)$ to $V(X)$; two such functions are adjacent in X^Y if they are compatible on Y. We say that X^Y is an *exponential graph*.

There is a complication—if f_0 is a homomorphism from Y to X, then f_0 is adjacent to itself in X^Y—and so in general X^Y has loops. In fact the number of loops is the number of homomorphisms from Y to X.

An example. Suppose Y is not bipartite. Then K_2^Y has no loops, and you may show that it is a disjoint union of copies of K_2. It follows that if Y is not bipartite and $Y \times Z$ is bipartite, then Z must be bipartite. There are easy direct proofs of this, but El-Zhar and Sauer used the exponential to prove the non-trivial result that if $\chi(Y) > 3$ and $\chi(Z) > 3$, then $\chi(Y \times Z) > 3$. A famous conjecture of Hedetniemi asserted that

$$\chi(Y \times Z) = \min\{\chi(Y), \chi(Z)\};$$

we now know that this is false.

1.4 The Homomorphic Product

A coclique in $X \square K_m$ corresponds to a set of m pairwise disjoint cocliques $X \square K_m$, and so $\alpha(X \square K_m)$ is the maximum size of an induced m-colourable subgraph of X. Equivalently $\alpha(X \square K_m)$ is the maximum size of an induced subgraph of X that admits a homomorphism to K_m. We introduce a product construction (due to Hell and Nesetril) that extends this observation.

The vertex set of the *homomorphic product* $X \ltimes Y$ of X and Y is

$$V(X) \times V(Y),$$

where (a,u) is adjacent to (b,v) if

- $a = b$, or
- $a \sim b$ and $u \not\simeq v$.

We use K_Y to denote the complete graph with vertex set $V(Y)$ and note that

$$A(X \ltimes Y) = A(X \,\square\, K_Y) + A(X \times \overline{Y})$$

If f is a function from $V(X)$ to $V(Y)$, its graph[3] is the subset

$$\{(a, \psi(a)) : a \in V(X)\}$$

of $V(X) \times V(Y)$.

A subset of $V(X) \times V(Y)$ is a relation from X to Y.

[3] this is the definition of graph from Calculus

1.4.1 Lemma. *A relation from X to Y is a function if and only if it induces a coclique in $X \,\square\, K_Y$.* □

1.4.2 Lemma. *Suppose X_1 is an induced subgraph of X and f is a function from $V(X_1)$ to $V(Y)$. Then f is a homomorphism if and only if its graph is a coclique in $X \ltimes Y$.*

2

Quantum Homomorphisms

2.1 Measurements

A *measurement* on the graph Y is a map φ from $V(Y)$ to the set of $d\times d$ projections such that $\sum_{u\in V(Y)}\varphi(u)=I$. We say that d is the *dimension* of the measurement.

2.1.1 Lemma. *If $P_1,\ldots,P_m$ are projections and $\sum_u P_u = I_d$, then $P_uP_v=0$ if $u\neq v$.*

Proof. We have

$$I=I^2=\Big(\sum_u P_u\Big)^2=\sum_u P_u+\sum_{u,v:u\neq v}P_uP_v.$$

As $\sum_u P_u = I$, this implies that

$$0=\operatorname{tr}(\sum_{u,v:u\neq v}P_uP_v)=\sum_{u,v:u\neq v}\operatorname{tr}(P_uP_v);$$

since projections are positive semidefinite, if $\operatorname{tr}(P_uP_v)=0$ then $P_uP_v=0$. □

We can extend this lemma: if $\sum_u P_u$ is idempotent, then $P_uP_v=0$ when $u\neq v$.

We say that measurements

$$(P_u)_{u\in V(Y)},\quad (Q_u)_{u\in V(Y)}$$

in Y are *compatible* relative to Y if, whenever u and v are non-adjacent vertices in Y, we have $P_uQ_v=0$. (This implies that $P_uQ_u=0$.) The *measurement graph* $\mathcal{M}(Y,d)$ is the graph with the d-dimensional measurements on Y as its vertices, with two measurements adjacent if and only if they are compatible relative to Y.

If P_1 and P_2 are two measurements based on Y, we define their *outer product* to be the $|V(Y)|\times|V(Y)|$ matrix M given by

$$M_{i,j}=\langle P_{1,i},P_{2,j}\rangle+\langle P_{2,i},P_{1,j}\rangle$$

Since the components of a measurement are positive semidefinite, we see that $M_{i,j}=0$ if and only if both $P_{1,i}P_{2,j}$ and $P_{2,i}P_{1,j}$ are zero.

2.1.2 Lemma. *Let P_1 and P_2 be two measurements of dimension d based on Y and let M be their outer product. Then P_1 and P_2 are adjacent in $\mathcal{M}_d(Y)$ if and only if $(J - A(Y)) \circ M = 0$.*

In general $\mathcal{M}(Y, d)$ is infinite. The case $d = 1$ is special.

2.1.3 Lemma. *If Y is a graph, then $Y \cong \mathcal{M}_1(Y)$.*

Proof. If $\sum_i P_i = 1$ then there is exactly one index j such that $P_j = 1$ and $P_i = 0$ if $i \neq j$. Hence the vertices of $\mathcal{M}_1(Y)$ can be identified with the standard basis vectors indexed by $V(Y)$. If e_u and e_v are two standard basis vectors, their outer product M is $e_i e_j^T + e_j e_i^T$, whence the lemma yields that e_i and e_j are adjacent in $\mathcal{M}_d(Y)$ if and only if $ij \in E(Y)$. □

If the matrices P_u for u in $V(Y)$ form a measurement, so do the matrices $P_u \otimes I_e$. It follows that $\mathcal{M}(Y, d)$ is (isomorphic to) an induced subgraph of $\mathcal{M}(Y, de)$.

2.2 Measurements and Homomorphisms

A *quantum homomorphism* from X to Y is a homomorphism from X to $\mathcal{M}(Y, d)$ for some d. We write $X \xrightarrow{q} Y$ to denote that there is a quantum homomorphism from X to Y. Thus $X \xrightarrow{q} Y$ if and only if $X \to \mathcal{M}(Y, d)$ (for some d).

We can represent a quantum homomorphism by a $|V(X)| \times |V(Y)|$ matrix M, where each row of M is a measurement on Y. The entries of M are $d \times d$ projections, thus M is a matrix over the ring $\mathrm{Mat}_{d\times d}(\mathbb{C})$. We may also view it as a block matrix of order $d|V(X)| \times d|V(Y)|$, in this case we denote it by $\widetilde{M}$. The defining properties of M are:

- Each row of M sums to I_d;
- If a and b are adjacent vertices in X and u and v are vertices in Y that are not adjacent, then $M_{a,u} M_{b,v} = 0$.

We introduce some operations on quantum homomorphisms. If the matrix M represents a quantum homomorphism from X to Y, then $M \otimes I_e$ also represents a quantum homomorphism from X to Y.

We show how to compose quantum homomorphisms. If M determines a quantum homomorphism from X to Y and N a quantum homomorphism from Y to Z, we define their *composition* $M \star N$ to be the matrix given by

$$(M \star N)_{a,z} = \sum_{u \in V(Y)} M_{a,u} \otimes N_{u,z}.$$

Because the Kronecker product is associative, composition is an associative operation. We leave the proof of the following as an exercise.

2.2.1 Theorem. *If M determines a quantum homomorphism from X to Y and N a quantum homomorphism from Y to Z, then $M \star N$ determines a quantum homomorphism from X to Z.* □

There is also a sum operation on quantum homomorphisms from X to Y. If M and N determine quantum homomorphisms from X to Y, their sum $M \boxplus N$ is given by

$$(M \boxplus N)_{a,u} = M_{a,u} \boxplus N_{a,u}.$$

The direct sum of quantum homomorphisms is again a quantum homomorphism (as you may verify).

Quantum homomorphisms with $d = 1$ are precisely the classical homomorphisms.

2.2.2 Lemma. *Let M determine a quantum homomorphism of dimension d from X to Y. If all entries of M commute, it is a direct sum of classical homomorphisms.*

Proof. The entries of M are Hermitian matrices and therefore if they commute, they are simultaneously diagonalizable. Since they are projections, their diagonalizations are 01-matrices. □

It is an interesting exercise to show that if $d = 2$, the entries of M must commute.

Next, suppose P is a $d \times d$ positive semidefinite matrix. If M represents a quantum homomorphism, let $\tau_P(M)$ be given by

$$(\tau_P(M))_{a,u} = \operatorname{tr}(PM_{a,u}).$$

If $P = I$, this may be viewed as a partial trace. If $P = RR^*$, then

$$\operatorname{tr}(PM) = \operatorname{tr}(RR^* M) = tr(R^* MR)$$

and therefore $\operatorname{tr}(PM)$ is real and non-negative. If we assume $\operatorname{tr}(P) = 1$, the entries of a row of $\tau_P(M)$ are non-negative reals summing to 1, i.e., they form a probability density on $V(Y)$. You should verify that

$$\tau_{P\oplus Q}(M \oplus N) = \tau_P(M) + \tau_Q(N)$$

and

$$\tau_{P\otimes Q}(M \star N) = \tau_P(M)\tau_Q(N).$$

This implies that τ_I is a functor.

In this section we have been precise and referred to our matrices of projections as "determining a quantum homomorphism". We plan to get sloppy and identify the quantum homomorphism with the matrix.

2.3 Products and Coproducts

We have a category with graphs as objects and quantum homomorphisms as arrows. This category has products and coproducts, as we are about to show.

If $X, Y \xrightarrow{q} Z$, then $(X \cup Y) \xrightarrow{q} Z$. For if $X \to \mathcal{M}(Z,d)$ and $Y \to \mathcal{M}(Z,e)$ then, since both $\mathcal{M}(Z,d)$ and $\mathcal{M}(Z,e)$ admit homomorphisms to $\mathcal{M}(Z,de)$, we have homomorphisms from X and Y to $\mathcal{M}(Z,de)$ and so $(X \cup Y) \xrightarrow{q} Z$. So our category has coproducts—they are the coproducts in the category of graphs.

2.3.1 Lemma. *If $\mathscr{P}$ is a measurement on X with dimension d and $\mathscr{Q}$ a measurement on Y with dimension e, then*

$$\mathscr{P} \otimes \mathscr{Q} := (P_a \otimes Q_u)_{a \in V(X), u \in V(Y)}$$

is a measurement on $X \times Y$ with dimension de. If $\mathscr{P}'$ and $\mathscr{Q}'$ are measurements on X and Y respectively, and $\mathscr{P} \sim \mathscr{P}'$ and $\mathscr{Q} \sim \mathscr{Q}'$, then $\mathscr{P} \otimes \mathscr{P}' \sim \mathscr{Q} \otimes \mathscr{Q}'$.

Proof. If $\mathscr{P}$ and $\mathscr{Q}$ are measurements on X and Y respectively, then the matrices $P_a \otimes Q_u$ form a measurement on $X \otimes Y$.

Assume $\mathscr{P}'$ and $\mathscr{Q}'$ are measurements on X and Y respectively and that $cP' \sim \mathscr{Q}'$. Suppose (a,u) and (b,v) are non-adjacent vertices in $X \times Y$. If $a \not\sim b$ then $P_a P'_b = 0$, if $u \not\sim v$ then $Q_u Q'_v = 0$ and, consequently,

$$(P_a \otimes Q_u)(P'_b \otimes Q'_v) = 0.$$

This shows that $\mathscr{P} \otimes \mathscr{P}' \sim \mathscr{Q} \otimes \mathscr{Q}'$. □

2.3.2 Corollary. *The product $\mathcal{M}(X,d) \times \mathcal{M}(Y,e)$ is isomorphic to a subgraph of $\mathcal{M}(X \times Y, de)$.* □

If $Z \xrightarrow{q} X$ and $Z \xrightarrow{q} Y$, then $Z \to \mathcal{M}(X,d)$ and $Z \to \mathcal{M}(Y,e)$ (for some d and e). Therefore

$$Z \to \mathcal{M}(X,d) \times \mathcal{M}(Y,e) \to \mathcal{M}(X \times Y, de).$$

It follows that our category has products, and these coincide with the products in the category of graphs.

2.4 Measuring States

A *state* is a positive semidefinite matrix with trace one. Let P be a quantum homomorphism from X to Y and let D be a state. We define the matrix $\langle P, D\rangle$ by

$$\langle P, D\rangle_{u,v} := \operatorname{tr}(P_{u,v} D);$$

this is a non-negative matrix with each row summing to 1. We say that $\langle P, D\rangle$ is obtained by *measuring* D using P.

2.4.1 Lemma. *If D and E are states and $P : X \xrightarrow{q} Y$ and $Q : Y \xrightarrow{q} Z$, then $\langle P \star Q, D \otimes E\rangle = \langle P, D\rangle \langle Q, E\rangle$.* □

2.4.2 Lemma. *If P and Q are quantum homomorphisms from X to Y, then*

$$\langle P \boxplus Q, D \oplus E\rangle = \langle P, D\rangle + \langle Q, E\rangle. \qquad \square$$

If P is a quantum automorphism, $\langle P, D\rangle$ is doubly stochastic.

2.4.3 Theorem. *If we measure a quantum permutation P using a density matrix D, then $\langle P, D\rangle$ is a doubly stochastic. If P is a quantum automorphism of X, then $\langle P, D\rangle$ commutes with $A(X)$.*

If a doubly stochastic matrix S commutes with $A(X)$, then X admits an equitable partition with cells that are not all singletons. Let Q be the normalized characteristic matrix of this partition. Then QQ^T commutes with A, which implies that X has eigenvectors that sum to zero on the cells of the partition. This implies that X is not controllable. Since almost all graphs are controllable, we conclude that the proportion of graphs on n vertices that admit a non-trivial quantum homomorphism goes to zero as $n \to \infty$.

2.5 Cliques and Colourings

Let P be a quantum homomorphism. If

$$0 = \sum_u P_{a,u} P_{b,u},$$

then

$$0 = \sum_u \operatorname{tr}(P_{a,u} P_{b,u}).$$

As the entries of P are positive semidefinite, $\operatorname{tr}(P_{a,u} P_{b,u}) \geq 0$ with equality if and only if $P_{a,u} P_{b,u} = 0$. We say that two rows of P are orthogonal if they are entrywise orthogonal. This yields the following.

2.5.1 Lemma. *Let P be a $|V(X)| \times m$ matrix of $d \times d$ projections. Then P determines a quantum homomorphism $X \xrightarrow{q} K_m$ if and only if whenever $a \sim b$, the a- and b-rows of P are orthogonal.* $\square$

Supose P is a quantum homomorphism from X to Y of index d. If $P_{a,u} = I_d$, and $v \neq u$, then $P_{a,v} = 0$; if $b \neq a$ we also have $P_{b,u} = 0$. So P has the form

$$\begin{pmatrix} I_d & 0 \\ 0 & P_1 \end{pmatrix}$$

where P_1 is a quantum homomorphism from $X \setminus a$ to $Y \setminus b$.

2.5.2 Theorem. *If there is a quantum homomorphism $X \xrightarrow{q} K_2$, then X is bipartite.*

Proof. Assume $P_{a,1} = R$. Then $P_{a,2} = I - R$.

Suppose $P_{b,1} = S$. If $a \sim b$, then $RS = 0$ and

$$0 = (I - R)(I - S) = I - R - S + RS = 1 - R - S$$

and hence $S = I - R$.

3

Quantum Colouring

3.1 Type-II Matrices

We use $W^{(-)}$ to denote the Schur inverse of a matrix W (which need not be square). We that an $n \times n$ matrix W is a *type-II* matrix if $WW^{-)T} = nI$. Hadamard matrices provide one class of type-II matrices. More generally a unitary matrix is type-II if and only if it is flat. For any nonzero complex number t, the matrix

$$W = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & t & -t \\ 1 & -1 & -t & t \end{pmatrix}$$

is type-II.

A *monomial matrix* is the product of a permutation matrix and an invertible diagonal matrix. The monomial matrices of a given order form a group. If M and N are monomial and W is type-II, then MWN is type-II. We say that MWN and W are equivalent. If W is type-II so is W^T, but in general W and W^T are not equivalent. If W_1 and W_2 are type-II matrices, so is $W_1 \otimes W_2$.

3.1.1 Lemma. *An $n \times n$ matrix W is type-II if and only if for any two diagonal matrices D_1 and D_2,*

$$\langle D_1, W^{-1} D_2 W \rangle = \frac{1}{n} \operatorname{tr}(D_1) \operatorname{tr}(D_2).$$

Proof. We have

$$\langle e_i e_i^T, W^{-1} e_j e_j^T W \rangle = \operatorname{tr}(e_i e_i^T W^{-1} e_j e_j^T W) = e_i^T W^{-1} e_j e_j^T W e_i = (W^{-1})_{i,j} W_{j,i},$$

and so our claim holds for $D_1 = e_i e_i^T$ and $D_2 = e_j e_j^T$ if and only if

$$(W^{-1})_{i,j} W_{j,i} = \frac{1}{n}.$$

It holds for all i and j if and only if $W^{-1} = \frac{1}{n} W^{(-1)T}$, i.e., if W is type-II. The result now follows by linearity. □

3.1.2 Corollary. *If W is type-II of order $n \times n$ and D is diagonal,*

$$(W^{-1}DW)_{i,i} = \frac{1}{n}\operatorname{tr}(D). \qquad \square$$

3.1.3 Lemma. *Suppose $P_1, \dots, P_k$ are pairwise orthogonal projections summing to I. If W is a $k \times k$ type-II matrix and we define*

$$U_i = \sum_j W_{i,j} P_i \qquad (i = 1, \dots, k),$$

then $U_1, \dots, U_k$ are invertible and

$$\sum_i P_i \otimes P_i = \sum_i U_i \otimes U_i^{-1}.$$

If W is unitary, so are $U_1, \dots, U_k$.

3.2 Orthogonality Graphs

We define $\mathcal{G}(d, r)$ to be the graph with vertices the complex $d \times d$ projections of rank r, with two projections P and Q adjacent if and only if they are orthogonal, i.e., if $PQ = 0$ or $\langle P, Q \rangle = 0$. We have

$$\|P - Q\|^2 = \langle P - Q, P - Q \rangle = 2r - 2\langle P, Q \rangle;$$

since $P, Q \succcurlyeq 0$ it follows that $\langle P, Q \rangle \geq 0$ and therefore two projections are orthogonal if they are at maximum distance.

A projection in $\mathcal{G}(d, r)$ that fixes e_1 has the form

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

where $Q \in \mathcal{G}(d-1, r-1)$; therefore $\mathcal{G}(d-1, r-1)$ is an induced subgraph of $\mathcal{G}(d, r)$.

The diagonal matrices in $\mathcal{G}(d, r)$ are 01-matrices and the subgraph they induce is the Kneser graph $K_{d:r}$.

We will most often use the graph $\mathcal{G}(d, 1)$. The subgraph of $\mathcal{G}(d, 1)$ induced by the flat projections will be denoted by $\mathcal{G}^\flat$. The least integer d such that a graph X admits a homomorphism into $\mathcal{G}(d, 1)$ is called the *orthogonal rank* of X, and is denoted by $\xi(X)$. The least integer d such that X admits a homomorphism into $\mathcal{G}^\flat(d)$ is the *flat orthogonal rank*, denoted $\xi^\flat(X)$.

3.3 Colourings from Projections

Let X be a graph with n vertices. A *quantum c-colouring* is an $n \times c$ matrix N such that $N_{u,i}$ is a $d \times d$ projection for each vertex u and $i = 1, \dots, c$ and:

(a) For each vertex u we have $\sum_i N_{u,i} = I_d$,

(b) If u and v are adjacent vertices, then $N_{u,i}N_{v,i} = 0$.

Condition (a) implies that the projections in a row are pairwise orthogonal. The minimum value of c for which a quantum c-coluring exists is the *quantum chromatic number* of X, denoted $\chi_q(X)$.

If the projectors $N_{u,i}$ each have rank r, we say we have a quantum rank-r colouring. In this case $cr = d$. It can be shown that if a quantum c-colouring exists, then there is a rank-r quantum c-colouring for some r. We will generally work with rank-r colourings.

A classical c-colouring is a quantum c-colouring (with $d = 1$): take N to be the characteristic matrix of the partition of $V(X)$ into colour classes. Also, it is not hard to show that if X admits a quantum 2-colouring, it is bipartite.

Assume X has a quantum c-coloring with $d \times d$ projections given by a matrix N. Define block-diagonal $nd \times nd$ matrices $P_1, \ldots, P_c$, where the j-th diagonal block of P_i is $N_{j,i}$. We observe that P_i is a projection and $\sum_i P_i = I$. (For a classical c-colouring, the matrices P_i are diagonal and 01.)

3.3.1 Lemma. *The projections $P_1, \ldots, P_c$ come from a quantum c-colouring if and only if*

$$\sum_{i=1}^{c} P_i(A \otimes I_d)P_i = 0. \qquad \square$$

If M is diagonal,

$$\sum_{i=1}^{c} P_i(M \otimes I_d)P_i = M \otimes I_d.$$

If M runs over the algebra of matrices of order $nd \times nd$, then the matrices

$$\sum_i P_i M P_i$$

form a subalgebra, and the map $M \mapsto \sum_i P_i M P_i$ is an orthogonal projection.

3.4 Rank-r Colourings and Unitary Derangements

Suppose $P_1, \ldots, P_k$ is sequence of pairwise orthogonal $d \times d$ projections with rank r, summing to I. Choose, for each i, a $d \times r$ matrix S_i such that the columns of S_i are orthonormal ($S_i^* S_i = I_r$). Since $P_i P_j = 0$ when $i \neq j$, we have $S_i^* S_j = 0$ when $i \neq j$. It follows that if U is the $d \times d$ matrix

$$U = \begin{pmatrix} S_1 & \ldots & S_k \end{pmatrix}$$

then $U^* U = I_d$, i.e., U is unitary. Thus our sequence of projections corresponds to a unitary matrix, along with a partition of its columns into submatrices of order $d \times r$.

Assume now that the matrix N determines a rank-r quantum c-colouring of X. Then each row of N gives rise to a partitioned $d \times d$ unitary matrix, with each row using the same partition. If U_a and U_b are the unitaries corresponding to adjacent vertices a and b, then $U_a^* U_b$ is a unitary matrix with c/r zero diagonal blocks of order $r \times r$. We will call such a matrix a *unitary derangement of rank* r.

Let $\mathscr{D}$ denote the set of unitary derangements of order $d \times d$ and rank r. Then $\mathscr{D}$ is closed under inversion, and so we may form the Cayley graph $X(U(d), \mathscr{D})$. We call this the *rank-r unitary derangements graph*, asnd we denote it by $\mathscr{U}\mathscr{D}(d, r)$. A graph Y has a quantum c-colouring of rank r if and only if there is a homomorphism from Y into $\mathscr{U}\mathscr{D}(d, r)$. (Here $d = cr$.)

There is classical analog in the rank-1 case. The symmetric group $\operatorname{Sym} d$ is a subgroup of $U(d)$, and a permutation in $\operatorname{Sym} d$ is a *derangement* if it has no fixed point. If $\mathscr{D}$ denotes the set of derangements, we have a Cayley graph $X(\operatorname{Sym} d, \mathscr{D})$. The permutations that fix a point i form a coclique in this Cayley graph of size $(d-1)!$. On the other hand, if L is a $d \times d$ Latin square, then each row of L determines a permutation in $\operatorname{Sym} d$ and the permutations corresponding to the rows of L form a clique in our Cayley graph of size d. In particular the chromatic number of our Cayley graph is d, and so $\chi(Y) \le d$ if and only if there is homomorphism from Y into the Cayley graph.

3.5 *Inequalities*

We will derive a number of inequalities between some of our parameters

3.5.1 Theorem. *We have homomorphisms*

$$\mathscr{G}^\flat(d) \to \mathscr{U}\mathscr{D}(d, 1) \to \mathscr{G}(d, 1).$$

Proof. Choose a flat unitary $d \times d$ matrix W and assume $zz^* \in \mathscr{G}^\flat(d)$. Let D_z denote the diagonal matrix formed from the first column of P, scaled to make it unitary. (This is possible because z is flat.) Then

$$\frac{1}{\sqrt{d}} D_z W$$

is unitary. If $yy^* \in \mathscr{G}^\flat(d)$ and D_y is unitary, then

$$(D_y W)^* D_z W = W^* D_y^* D_z W$$

and by Corollary 3.1.2, it follows that the diagonal entries of $W^* D_y^* D_z W$ are zero if $\langle y, z \rangle = 0$. We conclude that the map

$$z \mapsto \frac{1}{\sqrt{d}} D_z W$$

is a graph homomorphism.

The map

$$\nu : U \mapsto U^* e_1^T e_U$$

send a unitary matrix to a rank-1 projection. If $M, N \in U(d)$ and $M^* N$ is a unitary derangement, then

$$0 = (M^* N)_{1,1} = \langle Me_1, Ne_1 \rangle.$$

Therefore ν is a graph homomorphism. □

We can derive derive a chain of inequalities for our parameters.

3.5.2 Lemma. *For any graph X,*

$$\omega(X) \le \xi(X) \le \chi_q^{(1)}(X) \le \xi^\flat(X) \le \chi(X).$$

Proof. If projections P and Q are orthogonal, then their first columns Pe_1 and Qe_1 are orthogonal, and first inequality follows from this.

The second and third inequalities are consequences of the previous theorem.

Finally if N is the matrix a classical c-colouring, then the rows of N are unit vectors such that vectors associated to adjacent vertices are orthogonal, and so the final inequality holds. □

Consider the graph $H(d)$, with vertices the ± 1-vectors of length d, with two vectors adjacent if they are orthogonal. If d is odd, $H(d)$ is empty and if $d \cong 2$ (modulo 4), then it is bipartite. If $4 \mid d$, then by a result of Frankl and Rödl, that $\chi(H(d))$ increases exponentially with d. (By work of Newman we know that $\chi(H(d)) = d$ if and only if $d \in \{1, 2, 4, 8.\}$ Thus we have examples of graphs where there is an exponential gap between $\chi_q^{(1)}$ and χ.

3.5.3 Lemma. *If $\chi_q^{(1)}(X) = 3$, then $\chi(X) = 3$.*

Proof. A 3×3 unitary derangement must be a monomial matrix. Now work a bit. □

We also have that $\chi_{sv}(X) \le \xi(X)$, see [1].

[1]

3.6 Orthogonal Rank

Following Elphick and Wocjan, we derive lower bounds on the orthogonal rank $\xi(X)$ of a graph X.

We start with an orthogonal representation in terms of vectors, rather than projections. Let W be an $n \times k$ complex matrix such that $(W^* W) \circ A = 0$. Since the union of the subspaces $(We_i)^\perp$ is a proper subset of $\mathbb{C}^k$, there is a unitary matrix Q such that no entry in the first row of QW is zero and it follows that we may assume that all entries in the first row of W are equal to 1.

Let w_i denote the i-th row of W, and let D_i be the $n \times n$ diagonal matrix formed from w_i.

3.6.1 Lemma. *If the matrices $D_1, \dots, D_k$ are obtained from an orthogonal representation as above, then*

$$\sum_i D_i^* A D_i = 0.$$

Proof. We have

$$D_i^* A D_i = A \circ (w_i^*) w_i$$

and

$$\sum_{i=1}^k (w_i^*) w_i = W^* W.$$

Since $(W^* W) \circ A = 0$, the result follows. □

Because we have normalised W so that $e_1^T W = \mathbf{1}$, we have $D_1 = I$. Hence the lemma implies that

$$A = -\sum_{i=2}^k D_i^* A D_i. \tag{3.6.1}$$

3.6.2 Corollary. *For a graph X on n vertices,*

$$\xi(X) \ge 1 - \frac{\theta_1}{\theta_n}.$$

Proof. From Equation (3.6.1) we have

$$\theta_1(A) \le \sum_{i=2}^k -\theta_n(D_i^* A D_i) = -(k-1)\theta_n(A).$$ □

Note that if this bound is tight and z is an eigenvector for A with eigenvalue $\theta_1(A)$, then $D_i z$ is an eigenvector for A with eigenvalue θ_n. Hence the multiplicity of θ_n is at least $\xi(X) - 1$.

It is known that $\chi_{sv}(X) \le \xi(X)$ and that if X is a graph with n vertices, e edges and least eigenvalue τ, then

$$\chi_{vec}(X) \ge 1 - \frac{2e/n}{\tau}.$$

If X is k-regular then $2e/n = k$ and so we have a strengthening of the previous bound. If X is 1-homogeneous, then $\chi_{sv}(X) = \chi_{vec}(X) = 1 - k/\tau$.

There is also a form of inertia bound.

3.6.3 Corollary. *For a graph X on n vertices,*

$$\xi(X) \ge 1 + \max\left\{\frac{n^+}{n^-}, \frac{n^-}{n^+}\right\}.$$

Proof. Suppose A has spectral decomposition

$$A = \sum_r \theta_r E_r;$$

if we set

$$B = \sum_{r:\theta_r > 0} \theta_r E_r, \quad C = -\sum_{r:\theta_r < 0} \theta_r E_r,$$

then $B, C \succcurlyeq 0$ and $A = B - C$. Further define

$$F = \sum_{r:\theta_r<0} E_r.$$

Then F is a projection, $FB = 0$ and $FA = -C$. Referring back to Equation (3.6.1), we have

$$C - B = \sum_i \Delta_i A \Delta_i^*$$

(where $\Delta_i = U_1^* U_I$ and is unitary). Multiplying both sides by F, we get

$$C = \sum_i F\Delta_i(B-C)\Delta_i^* F = \sum_i F\Delta_i B\Delta_i^* F - \sum_i F\Delta_i C\Delta_i^* F.$$

Here the final sum is positive semidefinite, and so

$$C \preccurlyeq \sum_i F\Delta_i B\Delta_i^* F.$$

As the rank of each term in this sum is at most $\mathrm{rk}(B)$, it follows that

$$n^- \le (c-1)n^+,$$

whence the bound

$$\xi(X) \ge 1 + \max\left\{\frac{n^+}{n^-}, \frac{n^-}{n^+}\right\}. \qquad \square$$

3.7 *Orthogonal Rank and Rank-1 Colourings*

We follow Scarpa and Severini (arXiv:1106.0712v1).

Since the Cartesian product $X \square K_d$ contains copies of K_d, we have

$$\xi(X \square K_d) \le d.$$

When does equality hold? Assume that W is a $d \times nd$ matrix whose columns provide an orthgonal embedding of $X \square D$. Since the image of K_d must be an orthogonal set of vectors, we may assume that

$$W = \begin{pmatrix} U_1 & \dots & U_n \end{pmatrix}$$

where the $d \times d$ matrices $U_1, \dots, U_n$ are unitary.

Now

$$(W^*W) \circ (A \otimes I_d + I_n \otimes K_d) = 0.$$

We have $(W^*W) \circ (I_n \otimes K_d) = 0$ if and only if $U_i^* U_i = I$, i.e., U_i is unitary. We have $(W^*W) \circ (A \otimes I_d) = 0$ if and only if

$$(U_i^* U_j) \circ I = 0$$

whenever $ij \in E(X)$.

We conclude that $\xi(X \square K_d) = d$ if and only if $\xi_q^{(1)}(X \square K_d) = d$.

By way of comparison $\alpha(X \square K_d) = d$ if and only if $\chi(X) = d$.

4

Derangements

A *derangement* is a permutation of a set with no fixed point. If D denotes the set of derangements in $\mathrm{Sym}\, n$, then D is closed under inverses and does not contain the identity, so we may use D as the connection set for the Cayley graph $X(\mathrm{Sym}\, n, D)$; we denote this graph by $\mathscr{D}(n)$. We summarize some relevant properties of $\mathscr{D}(n)$.

4.0.1 Theorem. *We have:*

(a) *The maximum size of a clique in $\mathscr{D}(n)$ is n; cliques of size n correspond to $n \times n$ Latin squares.*

(b) *The maximum size of a coclique is $(n-1)!$; the cocliques of size $(n-1)!$ are cosets of the stabilizer of a point.*

(c) *The chromatic number of $\mathscr{D}(n)$ is n.* □

4.0.2 Corollary. *We have $\chi(X) \le n$ if and only if $X \to \mathscr{D}(n)$.* □

Two graphs X and Y are *homomorphically equivalent* if $X \to Y$ and $Y \to X$. The previous corollary may restated as the statement that $\mathscr{D}(n)$ and K_n are homomorphically equivalent.

Let us represent elements of $\mathrm{Sym}\, n$ by permutation matrices. The space of $n \times n$ complex matrices is an inner product space, with inner product

$$\langle M, N \rangle := \mathrm{tr}(M^* N).$$

If M is a permutation matrix, $M^* = M^{-1}$ and we see that if M and N are permutation matrices and $M^{-1}N$ represents a derangement, then $\langle M, N \rangle = 0$. Thus $\mathscr{D}(n)$ is an orthogonality graph.

4.1 Rank-1 Quantum Colourings and Unitary Derangements

Suppose M defines a quantum m-colouring of X, where the entries of M have rank one. Then the entries of M must be of order $m \times m$. If

$$P_1, \dots, P_m$$

are the projections in row i of M, then there are unit vectors $x_1, \dots, x_m$ such that

$$P_r = x_r x_r^*.$$

Since $P_r P_s = 0$ if $r \neq s$, the vectors $x_1, \dots, x_m$ are pairwise orthogonal, and therefore they form the columns of a unitary matrix, R say. If S is the unitary matrix corresponding to row j of M, then the condition $M_{i,r} M_{j,r} = 0$ holds for each r if and only the diagonal entries of $R^* S$ are all zero. Since R and S are unitary, so is $R^* S$.

We define a *unitary derangement* to be a unitary matrix with all diagonal entries zero. Any permutation matrix is unitary, and it is a unitary derangement if and only if the permutation it represents is a derangement. The inverse of a unitary derangement is its conjugate-transpose, and so it is again a unitary derangement. Hence we may define a Cayley graph $\mathcal{UD}(n)$ on the unitary group $U(d)$, with connection set the set of unitary derangements. Note that the derangement graph $\mathcal{D}(n)$ is an induced subgraph of $\mathcal{UD}(n)$.

4.1.1 Theorem. *A graph X has a rank-1 quantum n-colouring if and only if $X \to \mathcal{UD}(n)$.* □

4.1.2 Lemma. *If the matrices $M_1, \dots, M_n$ form a clique in $\mathcal{UD}(n)$, let $\mathcal{M}$ denote the $n \times n$ matrix of projections with*

$$\mathcal{M}_{i,j} = M_i e_j (M_i e_j)^*.$$

Then $\mathcal{M}$ is a rank-1 quantum n-colouring of K_n. □

A *quantum permutation* is an $n \times n$ matrix P whose entries are $d \times d$ projections, such that the projections in any row or column sum to I_d. Quantum permutations correspond to quantum n-colourings of K_n.[1]

If L is an $n \times n$ Latin square with entries from $\{1, \dots, n\}$ we can convert L to a quantum permutation: if $L_{i,j} = r$, replace the entry r by the projection $e_e e_r^T$.

If z is a unit vector in $\mathbb{C}^n$, then the unitary matrices M with i-th row equal to z form a coclique, for if $Me_i = Ne_i = z$ then

$$(M^* N)_{i,i} = e_i^T M^* N e_i = zz^* \neq 0$$

and $M^* N$ is not a derangement.

You may find it interesting to prove that $\chi_q^{(1)}(X) = 3$ if and only if $\chi(X) = 3$.

[1] Of course, classical n-colourings of K_n are permutations

4.2 Three Homomorphisms

We use homomorphisms to relate some of the parameters at hand. One observation is in order.

4.2.1 Lemma. *If W is a flat unitary matrix and D_1 and D_2 are diagonal matrices (all of the same order), then*

$$\langle D_1, W^* D_2 W\rangle = \operatorname{tr}(D_1)\operatorname{tr}(D_2). \qquad \square$$

4.2.2 Theorem. *We have homomorphisms as follows:*

$$K_n \to S^\flat(n) \to \mathcal{U}\mathcal{D}(n) \to S(n).$$

Proof. The n-cliques in $S^\flat(n)$ are exactly the flat unitary matrices of order $n \times n$. This takes care of the first homomorphism.

For the second, if $z \in \mathbb{C}^n$, let D_z be the diagonal matrix with

$$(D_z)_{i,i} = z_i.$$

If $z \in S^\flat(n)$, then D_z is unitary and the map

$$z \mapsto D_z W$$

takes elements of $S^\flat(n)$ to unitary matrices. Consider the matrix

$$Q = (D_y W)^* D_z W.$$

We have

$$Q_{i,i} = \operatorname{tr}(e_i e_i^T Q) = \langle e_i e_i^T, (D_y W)^* D_z W\rangle = \langle e_i e_i^T, W^* D_y^* D_z W\rangle$$

and, applying the lemma (with $D_1 = e_i e_i^T$), we deduce that

$$\langle e_i e_i^T, W^* D_y^* D_z W\rangle = \operatorname{tr}(W^* D_y^* D_z W) = \operatorname{tr}(D_y^* D_z) = \langle y, z\rangle.$$

Accordingly if y and z are orthogonal, then Q is a derangement.

The third homomorphism is again simple. As

$$\langle Me_1, Ne_1\rangle = (M^* N)_{1,1}$$

we may use the map $M \mapsto Me_1$ as the homomorphism. $\square$

4.2.3 Corollary. *For any graph X,*

$$\chi(X) \ge \xi^\flat(X) \ge \chi_q^{(1)}(X) \ge \xi(X). \qquad \square$$

4.3 Separating χ and χ_q

Let q be an odd prime power. The vertices of the Erdős-Rényi graph $ER(q)$ are the 1-dimensional subspaces of the 3-dimensional vector space over $GF(q)$; two subspaces spanned by nonzero vectors x and y are adjacent if $x^T y = 0$. (Note: this is not an Erdős-Rényi random graph.) We see that $ER(q)$ has $q^2 + q + 1$ vertices and each vertex has $q + 1$ neighbours but, unfortunately perhaps, there are $q + 1$ vertices with loops on them.

The graph we use is $ER(3)$, on 13 vertices. Each vertex is represented by a vector of length three with entries 0, 1 and -1. We normalize the vectors by assuming that the first non-zero entry is 1. Now we view these vectors as vectors over $\mathbb{R}$, and work with the orthogonality graph on these vectors. Denote it by Y. Clearly $\xi(Y) \le 3$.

Cameron et al. prove the following, using properties of the quaternions.

4.3.1 Lemma. *There is a homomorphism from $S_{\mathbb{R}}(4)$ into the subgraph of $\mathcal{UD}(4)$ induced by the real orthogonal matrices.* □

4.3.2 Corollary. *If $\xi_{\mathbb{R}}(x) \le 4$, then $\chi_q^{(1)}(X) \le 4$.* □

A direct computation shows that $\chi(Y) = 4$. Consider the cone $\hat{Y}$ over Y. Here $\xi_{\mathbb{R}}(\hat{Y}) \le 4$, whence $\chi_q(\hat{Y}) \le 4$. However $\chi(\hat{Y})$ must be five. Thus we have established that χ and χ_q can differ and, also, that a graph and its cone may have the same quantum chromatic number. We have not ruled out the possibility that $\chi_q(Y) = 3$, this is done in the oddities paper.

The *quaternions* $\mathbb{H}$ are the algebra over $\mathbb{R}$ generated by i, j and k, where

$$i^2 = j^2 = k^2 = -1, \quad ijk = -1.$$

If $z \in \mathbb{H}$ and $z = x_0 + ix_1 + jx_2 + kx_3$, then its *conjugate* z^* is

$$x_0 - ix_1 - jx_2 - kx_3.$$

The *norm* of z is $z^*z = x_0^2 + x_1^2 + x_2^2 + x_3^2$ and its *trace* is $z + z^* = 2x_0$. A *unit quaternion* is a quaternion with norm 1. A quaternion is *pure* if its trace is zero.

There is an obvious map from the vector space $\mathbb{R}^4$ to the algebra $\mathbb{H}$ which takes unit vectors in $\mathbb{R}^4$ to quaternions with norm 1. Denote it by q.

4.3.3 Lemma. *If $x, y \in \mathbb{R}^4$, then*

$$\langle x, y \rangle = \operatorname{tr}(q(x)^* q(y)).$$

In particular, $\langle x, y \rangle = 0$ if and only if $q(x)^* q(y)$ is pure.

If $a \in \mathbb{H}$, then we have a map L_a from $\mathbb{H}$ to itself, given by

$$L_a(z) = az.$$

Then L_a is $\mathbb{R}$-linear and

$$(L_a(z))^* L_a z = a^* a z^* z$$

and so if a has norm 1, then L_a is norm preserving. This gives an isomorphism from the group of unit quaternions into $O(4)$, the real orthogonal group.

4.3.4 Lemma. *Relative to the ordered basis* $1, i, j, k$*, the matrix representing* L_a *is*

$$\begin{pmatrix} a_0 & -a_1 & -a_2 & -a_3 \\ a_1 & a_0 & -a_3 & -a_2 \\ a_2 & a_3 & a_0 & -a_1 \\ a_3 & -a_2 & a_1 & a_0 \end{pmatrix}.$$

4.3.5 Corollary. *The matrix representing* L_a *is an orthogonal derangement if and only if* a *is pure.*

4.3.1 More Derangements

4.3.6 Theorem. *The orthogonal derangement graph* $\mathcal{OD}(4)$ *is homomorphically equivalent to* $\Omega_{\mathbb{R}}(4)$*.*

Proof.

1. If x, y in $\mathbb{R}^4$ are orthogonal, $q(x)^* q(y)$ is a pure quaternion.
2. $L_a L_b = L_{ab}$ (associativity).
3. If $q(x)^* q(y)$ is pure, then $L_{q(x)}^T L_{q(y)}$ is a derangement.

4.4 Derangements of Index k

We have seen that rank-1 colourings give rise to unitary derangements. What of rank-k colourings?

A $d \times d$ projection P of rank k can be written as $P = UU^*$, where U is $d \times k$ and its columns of are an orthonormal basis for $\operatorname{im}(P)$. So $U^* U = I_k$. If the matrix M represents a rank-k quantum m-colouring of X, there are $d \times k$ matrices $U_{a,i}$ (for $a \in V(X)$ and $i = 1 \ldots, m$) such that

$$U_{a,i}^* U_{a,i} = I_k, \quad U_{a,i} U_{a,i}^* = M_{a,i}.$$

We see that if $i \neq j$, then $U_{a,i}^* U_{a,j} = 0$ and if $ab \in E(X)$, then $U_{a,i}^* U_{b,i} = 0$. Let $\mathcal{U}$ be the matrix with ai-entry equal to $U_{a,i}$. Since $mk = d$, each row of $\mathcal{U}$ is a $d \times d$ unitary matrix. If $ab \in E(X)$, then

$$\begin{pmatrix} U_{a,1} & \ldots & U_{a,m} \end{pmatrix}^* \begin{pmatrix} U_{b,1} & \ldots & U_{b,m} \end{pmatrix}$$

is a unitary matrix of order $mk \times mk$ with k diagonal blocks of zeros.

We define a unitary matrix M to be a *unitary derangement of index k* if it has order $mk \times mk$ and

$$M \circ (I_m \otimes J_k) = 0.$$

(If $k = 1$ we recover our previous derangements.) We can apply this term to permutation matrices, since they are unitary, and we will refer to them simply as *derangements of index k*. Since the set of $mk \times mk$ unitary derangements with index k is closed under conjugate transpose and does not contain the identity, we can use it as the connection set for a Cayley graph for the full unitary group; if $n = km$, we denote it by $\mathcal{UD}_k(m)$.

4.4.1 Theorem. *A graph X on mk vertices has a rank-k quantum m-colouring if and only if there is a homomorphism $X \to \mathcal{UD}_k(m)$.* □

If M is a unitary derangement (of index one) and Q is unitary of order $k \times k$, then $M \otimes Q$ is a unitary derangement of index k.

4.5 Grassmann Graphs

The *Grassmann graph* $Gr(d,k)$ is the graph with the k-dimensional subspaces of $\mathbb{C}^d$ as vertices, with two subspaces adjacent if they are orthogonal. We may, and will, choose to represent the vertices of $Gr(d,k)$ by $d \times d$ projections of rank k. If P and Q are two such projections, then

$$\|P-Q\|^2 = \langle P-Q, P-Q\rangle = \operatorname{tr}(P+Q-PQ-QP) = 2k-2\langle P,Q\rangle.$$

Hence P and Q are at maximum distance if and only if they are orthogonal. (Since P and Q are positive semidefinite, $\langle P,Q\rangle \geq 0$.) Consequently we may view $Gr(d,k)$ as an analog of the Kneser graph $K_{d:k}$. Since the fractional chromatic number of a graph is determined by homomorphisms into Kneser graphs this suggests, correctly, that homomorphisms to Grassmann graphs will provide a quantum analog to fractional chromatic number.

4.5.1 Theorem. *There is a homomorphism $\mathcal{UD}_k(m) \to Gr(mk,k)$.*

Proof. Define

$$D = \begin{pmatrix} I_k & 0 \\ 0 & 0 \end{pmatrix}.$$

If M is a $md \times md$ unitary matrix, then

$$MDM^*$$

represents orthogonal projection onto the column space of MD, i.e., onto the span of the first k columns of M. If N is a second $md \times md$ unitary matrix, then

$$MDM^*NDN^* = 0$$

if and only if

$$DM^*ND = 0.$$

Hence the projections MDM^* and NDN^* are orthogonal if M^*N is a unitary derangement of index k, and this proves the theorem. □

If M represents a rank-r quantum m-colouring of X, each column of M provides a homomorphism from X into $Gr(mr,r)$.

5

Type-II Matrices

5.1 Definitions

If M and N are $m \times m$ matrices, their *Schur product* is the $m \times n$ matrix $M \circ N$ defined by

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

This is a commutative associative product with the all-ones matrix J as multiplicative identity. If no entry of M is zero, we define the matrix $M^{(-)}$ by

$$(M^{(-)})_{i,j} := M_{i,j}^{-1}$$

and call it the *Schur inverse* of M; clearly $M \circ M^{(-)} = J$. If M is a Schr invertible matrix we define

$$M_{i/j} := (Me_i) \circ (Me_j)^{(-)}.$$

Thus $M_{i/j}$ is the ration of the i-th and j-th columns of M.

An $n \times n$ complex matrix w is a *type-II matrix* if it is Schur invertible and

$$WW^{(-)T} = nI$$

Any Hadamard matrix is a type-II matrix, as is the character table of an abelian group. If W_1 and W_2 are type-II, so is the Kronecker product $W_1 \otimes W_2$. Two type-II matrices are *equivalent* if one can be obtained from the other by some combination of:

(a) permutations of rows and or columns,

(b) pre- or post-multiplication by invertible diagonal matrices.

If W is type-II, so is its transpose W^T, but in general W and W^T are not equivalent.

Our next result introduces an important class of type-II matrices. We say that a complex matrix is *flat* if its entries all have the same absolute value.

5.1.1 Lemma. *Suppose W is a square Schur-invertible matrix. Then any two of the following statements imply the third:*

(a) W *is type-II.*

(b) W *is flat.*

(c) W *is unitary.*

A flat unitary matrix is commonly referred to as a complex Hadamard matrix. The examples of type-II matrices we offered earlier are flat.

5.2 The Nomura Algebra

To each $m \times n$ Schur-invertible matrix W we associate its *Nomura algebra*, defined as the set of $m \times m$ matrices M such that each ratio $W_{i/j}$ is an eigenvector. Hence M lies in the Nomura algebra of W if and only if there are scalars $\Theta_{i,j}(M)$ such that

$$MW_{i/j} = \Theta_{i,j(M)} W_{i/j}.$$

We denote this algebra by $\mathcal{N}_W$. It contains the identity matrix, so it is at least not empty.

5.2.1 Lemma. *A square Schur-invertible matrix* W *is type-II if and only if* $J \in \mathcal{N}_W$. □

So if W is type-II, the dimension of its Nomura algebra is at least two.

There is a non-trivial class of examples based on finte abelian groups. Assume G is a finite abelian group of order n, given by $n \times n$ permutation matrices, and let W be its character table, with rows indexed by group elements and columns by characters. Then $W_{i/j}$ is a character of G, and therefore $\mathcal{N}_W$ consists of the matrices M for which there is a diagonal matrix D such that $MW = WD$. It is not hard to verify that all permutation matrices in G belomg to $\mathcal{N}_W$.

It is surprisingly difficult to provide examples of type-II matrices the dimension of the Nomura algebra is great than two. We can use products to get examples which we deem trivial: It can be proved that if W_1 and W_2 are type-II matrices, then

$$\mathcal{N}_{W_1 \otimes W_2} \cong \mathcal{N}_{W_1} \otimes \mathcal{N}_{W_2}.$$

Hence if W is the Kronecker prodiuct of k type-II matrices,

$$\dim(\mathcal{N}_W) \geq 2^k.$$

A type-II matrix W is a *spin model* if $W \in \mathcal{N}_W$. Spin models are important becuase they give rise to link invariants. Abelian group provide examples where the type-matrices are flat ; the only known examples where the type-II matrix is flat is based on the Higman-Sims graph (die to Jaeger [1]) 1
and a family due to Nomura [2] bases on Hadamard matrices. 2

5.3 Quantum Automorphisms

A *quantum permutation* P is an $n \times n$ matrix such that each entry is a $d \times d$ projection, and the projections in each row and column sum to I_d. We prefer to view P as a matrix over the ring of $d \times d$ matrices but, occasionally it is convenient to view it as an $nd \times nd$ matrix with blocks of size $d \times d$. In this case we will write $\tilde{P}$ to warn the reader of the change of viewpoint.

Note that if $Q_1, \ldots, Q_k$ are projections and $\sum_i Q_i = I$, then $Q_i Q_j = 0$ when $i \neq j$. If the entries in a quantum permutation P all have rank one, then P is also known as a *quantum Latin square*.

5.3.1 Lemma. *Suppose P is an $n \times n$ quantum unitary with $d \times d$ projections as entries. Then $\tilde{P}$ is unitary.*

Proof. Easy exercise. □

An important consequence of this result is that P and $\tilde{P}$ are invertible.

Following Roberson et al [3], we define two graphs X and Y on n vertices to be *quantum isomorphic* if there is a quantum permutation P of order $n \times n$, with entries projections of order $d \times d$, such that 3

$$(A(X) \otimes I_d)\tilde{P} = \tilde{P}(A(Y) \otimes I_d).$$

If $X = Y$, we have a *quantum automorphism* of X. Since P is unitary, the matrices $A(X) \otimes I$ and $A(Y) \otimes I$ are similar, and so we see that quantum isomorphic graphs are cospectral. We'll see that more is true, but there are graphs that are quantum isomorphic but not isomorphic. (See [4].) 4

An automorphism of the graph X on n vertices can be specified by an $n \times n$ permutation matrix Q such that $QA = AQ$. Then $Q \otimes I$ and $A \otimes I$ commute, and we see that any automorphism of a graph gives rise to quantum automorphism,

5.3.2 Lemma. *If P is a quantum permutation, $\tilde{P}$ commutes with $J \otimes I_d$.* □

This result is easy to prove, and is left to the reader. One consequence of it is that quantum isomorphic graphs are cospectral with cospectral complements.

Our next results holds provided the entries in any row of P satisfy

$$P_{i,j} P_{i,k} = \delta_{j,k} P_{i,j};$$

they do not need to be projections.

5.3.3 Lemma. *If P is a quantum permutation and $\tilde{P}$ commutes with $M \otimes I$ and $N \otimes I$, it commutes with $(M \circ N) \otimes I$.*

Proof. The ij-block of $(M \otimes I)\tilde{P}$ is

$$\sum_r M_{i,r} P_{r,j}$$

and, by hypothesis, this is equal to the ij-block of $\tilde{P}(M \otimes I)$:

$$\sum_s M_{s,j} P_{i,s}.$$

We have

$$\sum_r M_{i,r} P_{r,j} \sum_s N_{i,s} P_{s,j} = \sum_r (M_{i,r} N_{i,r}) P_{r,j}$$

where the right side is the ij-block of $((M \circ N) \otimes I)\tilde{P}$. Similarly

$$\sum_r M_{r,j} P_{i,r} \sum_r N_{r,j} P_{i,r} = \sum_r (M_{r,j} N_{r,j}) P_{i,r}$$

where the right side is the ij-block of $\tilde{P}((M \circ N) \otimes I)$. Since the left sides of the previous pair of equations are equal, our result follows. □

5.3.4 Lemma. *Let P be a quantum permutation. The set of matrices M such that $M \otimes I$ commutes with $\tilde{P}$ is $*$-closed.*

Proof. Since the entries of P are Hermitian, we have

$$(\tilde{P}(M^* \otimes I))_{x,y} = \sum_r P_{x,r} M^*_{r,y} = \sum_r \left(P_{x,r} M_{r,y}\right)^* = \left((\tilde{P}(M \otimes I))_{x,y}\right)^*$$

and, if P and $M \otimes I$ commute, then

$$\left((\tilde{P}(M \otimes I))_{x,y}\right)^* = ((M^* \otimes I)\tilde{P})_{x,y}.$$

It follows that if $M \otimes I$ commutes with $\tilde{P}$, so does $M^* \otimes I$. □

From the previous two lemmas we see that the set of matrices M such that $\tilde{P}$ commutes with $(M \otimes I)$ is a coherent algebra.

5.4 The Matrix of Idempotents of a Type-II Matrix

We describe an operation on type-II matrices which we can use to construct quantum permutations. Assume W is an $n \times n$ type-II matrix and, for each i and j, define a rank-1 matrix $\mathcal{Y}_{i,j}$ by

$$Y_{i,j} := \frac{1}{n} W_{i/j} (W_{j/i})^T.$$

Let $\mathcal{Y}_W$ denote the $n \times n$ matrix with ij-entry equal to $Y_{i,j}$ (for all i and j). We call it the *matrix of idempotents* of W.

We observe that

$$Y_{i,i} = \frac{1}{n} J$$

and

$$Y_{i,j}^T = Y_{j,i}.$$

The latter implies that $\mathcal{Y}_W$ is symmetric. Further

$$Y_{i,j}^{(-)} = n W_{j/i} (W_{i/j})^T = n^2 Y_{j,i}.$$

If $\mathscr{Y}^\tau$ denotes the matrix we get by replacing each entry of $\mathscr{Y}$ by its transpose (i.e., the partial transpose of $\mathscr{Y}$), then

$$\mathscr{Y}^\tau = \frac{1}{n}\mathscr{Y}^{(-)}.$$

Finally, if W is flat, then $Y_{i,j}$ is Hermitian.

5.4.1 Theorem. *Let $\mathscr{Y}$ be the matrix of idempotents of the $n \times n$ type-II matrix W. Then each row and column of $\mathscr{Y}$ sums to I.*

Proof. Let $\partial_i(M)$ denote the diagonal matrix such that $(\partial_i(M))_{r,r} = (Me_i)_r$. We have

$$n\sum_j Y_{i,j} = \sum_j W_{i/j}(W_{j/i})^T = \partial_i(W)\left(\sum_j (We_j)^{(-)}(We_j)^T\right)\partial_i(W)^{-1}.$$

Here the inner sum is equal to

$$W^{(-)}W^T = (WW^{(-)T})^T = nI.$$

Since $\mathscr{Y}$ is symmetric, the result follows. □

Let S be the endomorphism of $\mathbb{C}^n \otimes \mathbb{C}^n$ that sends $u \otimes v$ to $v \otimes u$. Note that $S^2 = I$ and S is a permutation matrix.

5.4.2 Theorem. *If W is a type-II matrix, its matrix of idempotents $\mathscr{Y}$ is a type-II matrix. If W is flat, then $\mathscr{Y}$ is flat and is a quantum permutation.*

Proof. For fixed i, the vectors We_j form a basis of $\mathbb{C}^n$ and the vectors $n^{-1}(We_j)^{(-)}$ form a basis dual to this. Hence the matrices

$$\frac{1}{n}(We_j)^{(-1)}(We_j)^T$$

are pairwise orthogonal idempotents and sum to I. Therefore for fixed i the matrices $F_{i,j}$ are pairwise orthogonal idempotents that sum to I.

Since $\mathscr{Y}^T = \mathscr{Y}$, it also follows that each column of $\mathscr{Y}$ consists of pairwise orthogonal idempotents that sum to I. If W is flat, then $Y_{i,j}$ is Hermitian. □

5.4.3 Corollary. *If W is a Hadamard matrix, $\mathscr{Y}_W$ is a Hadamard matrix of Bush type.* □

5.4.4 Lemma. *If W is type-II, then $\mathscr{Y}_{W^T} = S\mathscr{Y}_W S$.*

Proof. We have

$$n(Y_{i,j})_{r,s} = \frac{W_{r,i}}{W_{r,j}}\frac{W_{s,j}}{W_{s,i}} = \frac{W_{r,i}}{W_{s,i}}\frac{W_{s,j}}{W_{r,j}} = \frac{W^T_{i,r}}{W^T_{i,s}}\frac{W^T_{j,s}}{W^T_{j,r}} = n(Y_{r,s}(W^T))_{i,j}.$$

Here the left hand and right hand terms are equal respectively to

$$(e_i \otimes e_r)^T\mathscr{Y}_W(e_j \otimes e_s), \qquad (e_r \otimes e_i)^T\mathscr{Y}(e_s \otimes e_j)$$

and the result follows. □

5.5 A Nomura Algebra is Schur-Closed

Let W be a type-II matrix. Recall that if $M \in \mathcal{N}_W$, then $\Theta_{i,j}(M)$ is the eigenvalue of M on the eigenvector $W_{i/j}$. Accordingly we define $\Theta_W(M)$ to be the matrix with

$$(\Theta_W(M))_{i,j} = \Theta_{i,j}(M);$$

it is the *matrix of eigenvalues* of M. Clearly, if $M, N \in \mathcal{N}_W$, then

$$\Theta_W(MN) = \Theta_W(M) \circ \Theta_W(N).$$

If M and N are square matrices of the same order, their Lie bracket is

$$[M,N] := MN - NM.$$

Obviously $[M,N] = 0$ if and only if M and N commute (and this is the only property of the Lie bracket that we will use.)

5.5.1 Theorem. *Let W by type-II and let $\mathscr{Y}$ be its matrix of idempotents. Then*

$$\mathcal{N}_W = \{M : [I \otimes M, \mathscr{Y}_W] = 0\},$$

and

$$\mathcal{N}_{W^T} = \{N : [N \otimes I, \mathscr{Y}_W] = 0\}.$$

Proof. We have that $[I \otimes M, \mathscr{Y}] = 0$ if and only if $[M, Y_{i,j}] = 0$ for all i and j. Now M commutes with a rank-1 matrix uv^* if and only if u is a right eigenvector for M. Hence $[M, Y_{i,j}] = 0$ for fixed i and all j if and only if $M \in \mathcal{N}_W$.

For the second claim,

$$S((N \otimes I)\mathscr{Y}_W)S = (I \otimes N)\mathscr{Y}_{W^T},$$

from which the assertion follows. □

5.5.2 Corollary. *If W is a type-II matrix, then $\mathcal{N}_W$ is Schur-closed.* □

If we show that $\mathcal{N}_W$ is closed under transpose, it will follow that $\mathcal{N}_W$ is the Bose-Mesner algebra of an association scheme. Similarly $\mathcal{N}_{W^T}$ will be a Bose-Mesner algebra; the relation between these two algebras is described in the following theorem, which we would like to be able to prove using the machinery at hand.

We have

$$(M \otimes I)\mathscr{Y} = (\Theta(M) \otimes J) \circ \mathscr{Y}.$$

5.5.3 Theorem (Nomura)**.** *If W is a type-II matrix of order $n \times n$, then*

$$\Theta_W(M) \in \mathcal{N}_{W^T}$$

and

$$\Theta_W(M \circ N) = \frac{1}{n}\Theta_W(M)\Theta_W(N)$$