Quantum independence and chromatic numbers

by

Mariia Sobchuk

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I hereby declare that I am the sole author of this thesis.

This is a true copy of the thesis, including any required final revisions, as accepted by my examiners.

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Abstract

In this thesis we are studying the cases when quantum independence and quantum chromatic numbers coincide with or differ from their classical counterparts. Knowing about the relation of chromatic numbers separation to the projective Kochen-Specker sets, we found an analogous characterisation for the independence numbers case. Additionally, all the graphs that we studied that had known quantum parameters exhibited both the separation between the classical and quantum independence numbers and the separation between the classical and quantum chromatic numbers. This observation and the Kochen-Specker connection suggested the possibility of the chromatic and independence numbers separations occurring simultaneously. We have disproved this idea with a counterexample. Furthermore, we generalised Manĉinska-Roberson's example of the chromatic numbers separation to an infinite family. We investigate some known instances with strictly larger quantum independence numbers in-depth, find a more general description and generalise Piovesan's example. Using the Lovász theta bound, we prove that there is no separation between the independence numbers in bipartite and perfect graphs. We also show that there is no separation when the classical independence number is two; and that the cone over a graph has the same quantum independence number as the underlying graph.

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Contents

Chapter 1

Introduction

The terms coclique and chromatic number became classical in graph theory over their more than 70 year long history. On the other hand, their quantum analogues appeared recently, with the first instance of quantum chromatic number generally attributed to the paper Cameron, Montanaro, Newman, Severini and Winter [7] published in 2007. The theory is captivating, as it shines new light on well-favoured graph theoretical properties, and draws subtle connections between Physics and Mathematics.

There have been two main directions of research in this area: one is to explore the difference of the quantum world and classical through Physical concepts and another one is to do so with Mathematical ideas. A lot of progress has been made by Mančinska, Roberson and Scarpa by 2013, when coincidentally they all published their theses [19], [26] and [27]. More recently, in 2016, interesting new results come from Piovesan's thesis [23]. Before learning how our work builds on their contributions, we first introduce the definitions of the quantum chromatic number and quantum independence number.

Throughout the thesis we use standard trace matrix inner product. For the matrices $P, Q \in \mathbb{C}^{n\times n}$ we have

$$\langle P, Q\rangle = \mathrm{tr} P^* Q.$$

Definition. For a graph X, the *quantum chromatic number* $\chi_q(X)$ is the minimum integer s for which there exist a $|V(X)|\times s$ block matrix P such that

$P^{(u,i)} \in \mathbb{C}^{d\times d}$ is a projection, and its entries satisfy the following conditions:

$$\sum_{i\in 1,\dots,s} P^{(u,i)} = I_d \text{ for all } u \in V(X)$$
$$\langle P^{(u,i)}, P^{(v,i)}\rangle = 0 \text{ for all } uv \in E(X) \text{ and } i = 1, ..., s$$

To get the intuition for this definition, let the entries of the matrix P be 1×1 projections, in other words integers 0 or 1. Given a classical colouring, let the ij-th entry $P^{(u,i)}$ be 1 if the vertex u is coloured colour i. In this case, P becomes a usual characteristic matrix of a classical colouring. Immediately, it follows that

$$\chi_q(X) \le \chi(X)$$

for any graph X.

Definition. For a graph X, the *quantum coclique number* $\alpha_q(X)$ is the maximum integer t for which there exist a $|V(X)| \times t$ block matrix P with $P^{(u,i)} \in \mathbb{C}^{d\times d}$, a projection such that

- $\sum_{v\in V(X)} P^{(u,i)} = I_d$ for all $i = 1, ..., t$
- $P^{(u,i)}P^{(v,j)} = 0$ for any $uv \in E(G)$ for all $i, j = 1, ..., t$
- $P^{(u,i)}P^{(u,j)} = 0$ for any $i \ne j$ for all $i, j = 1, ..., t$ and $u \in V(X)$

To get a better feeling for the definition, considering 1×1 projections may help again. Let us assume, vertices in the α-coclique are labelled as $1, ..., \alpha$, and making the $P^{(u,i)}$ entry one if u is the i^{th} vertex of the coclique. Again, P is now just a characteristic matrix of a coclique. Similarly, this shows that for any graph X we have

$$\alpha(X) \ge \alpha_q(X).$$

The idea is that if the dimension of the projections is greater than one, these two definitions generalise the classical parameters. The purpose of this thesis has been studying the known examples of the results on separation and generalising them.

One way to look at this topic is as in Roberson's thesis [26], where he views the quantum graph parameters through the lens of quantum homomorphisms, just as the classical chromatic and independence numbers can be defined in terms of classical homomorphisms. He finds a pair of graphs between which there is a quantum homomorphism, but no classical one which yields a graph with the separation between the classical and quantum independence numbers.

In the next thesis, Piovesan [23] gives an example of an orthogonality graph of a Kochen-Specker set, a construction that we call a Kochen-Specker graph, which exhibits the separation between the classical and quantum independence numbers.

Roberson and Mančinska [20] came up with the example of a graph on 14 vertices, a cone over a graph on 13 vertices, G_{13}, where the two chromatic numbers differ. Remarkably, G_{13} was an orthogonality graph of a Kochen-Specker set. A *Kochen-Specker set* is a set of vectors in a Hilbert space, such that it is impossible to pick one vector from each basis without picking two orthogonal ones. We will see them coming up again soon.

There are instances of separations in large graphs, for example in [27], but we are looking for generalising examples, possibly for new infinite families. We study smaller graphs.

There have been known infinite families of graphs where either $\chi > \chi_q$ [4] or $\alpha < \alpha_q$ [27]. The former construction involves Hadamard graphs and the latter builds on the chromatic separation to yield the independence numbers difference. In this thesis, we show that all Erdős-Rényi graphs give rise to the graphs whose quantum chromatic number is strictly larger than its classical counterparts (more detail can be found in4.4.1). Using Scarpa's construction this yields more graphs with the independence numbers gap. This new example builds on Mančinska and Roberson's work in [20]. We observed that G_{13} is an Erdős-Rényi graph [11] and defined an embedding of the Erdős-Rényi graph into $\mathbb{R}^3$. Applying Mančinska and Roberson's technique, we proved that such embedded graphs have the chromatic numbers separation.

We have also come up with a new graph on 120 vertices exhibiting separation between the quantum and classical independence numbers. For this we first observed [11] that the graph from Piovesan's thesis [23] is a Cayley graph. To understand the relation better, we have found an explicit homomorphism which to our surprise used Quaternion algebra. Changing the underlying group and using Quaternions, we have come up with the abovementioned 120-vertex graph.

On the physical side, Scarpa and Mančinska determined the condition for the sets of projections defining the quantum chromatic number to guarantee the separation with the classical chromatic number in terms of the Kochen-Specker sets.

1.0.1 Theorem. *For all graphs G, we have that $c = \chi_q(G) < \chi(G)$ if and only if the entries $\{P^{(v,a)}\}_{v \in V(G), a \in [c]}$ of the $|V(G)| \times c$ quantum chromatic matrix P is a projective KS set.*

Encountering Kochen-Specker sets so very often led us to wonder if a similar condition can be proved for the projections defining the quantum independence number, resulting in the next theorem.

1.0.2 Theorem. *For all graphs G, we have that $k = \alpha_q(G) > \alpha(G)$ if and only if the entries $\{P^{(v,a)}\}_{v \in V(G), a \in [k]}$ of the $|V(G)| \times k$ quantum chromatic matrix P form a projective KS set.*

And while the separation examples are relatively scarce and difficult to find, the instances of results which echo the classical intuition are of interest as well. Using the known bounds, we observed that bipartite and perfect graphs exhibit no separation. While G_{14} has the gap for the chromatic numbers, Lovász theta bound that was within one from $\alpha(G_{13})$, broke our hopes of G_{13} or its cone of exhibiting the difference between the independence numbers.

In analogy to the result of being quantum bipartite being equivalent to being classically bipartite [7], we proved the following:

1.0.3 Lemma. *If $\alpha(G) = 2$, then $\alpha_q(G) = 2$.*

Finally, as one would expect:

1.0.4 Lemma. *Consider a graph X. If $X \cup \{v\}$ is obtained by adding an apex vertex v to X, then $\alpha_q(X) = \alpha_q(X \cup \{v\})$.*

Since we are working a lot with quantum measurements, we will present some Physical background about the quantum measurement postulate. Additionally, we include the history of the Kochen-Specker theorem, as it also plays an important role in this thesis.

Chapter 2

Homomorphisms

This thesis is a study of the quantum chromatic number and the quantum independence number of a graph. Logically, we will start with the classical background and gradually relate it to the quantum notions with the help of the language of homomorphisms.

It is well known that the chromatic number of a graph X can be expressed in terms of the existence of a homomorphism from X into a complete graph. Moreover, finding the coclique number is equivalent to finding a homomorphism from $K_{\alpha(X)}$ to the complement of the original graph $\overline{X}$. In this chapter, we will review these concepts.

Mančinska and Roberson [21], [26] defined the quantum chromatic and independence numbers and generalised homomorphisms to quantum homomorphisms. Originally, this had been done in terms of games. However, since they are not the main focus of this thesis, the reader can get acquainted with the games definition in the appendix to this chapter. We will use the newer definition in terms of projections.

We will define orthogonal graph representation and learn two theorems on the quantum chromatic number, which will demonstrate the importance of this graph representation for the subject.

Finally, since projections are central in this area, there is a brief overview of linear algebraic tools reoccurring throughout the proofs in the end.

2.1 Classical definitions

Chromatic number and independence number are central notions in graph theory.

Chromatic number is a famous graph parameter. It is usually defined as the least integer r such that each vertex of X can be assigned one of r colours such that adjacent vertices receive different colours.

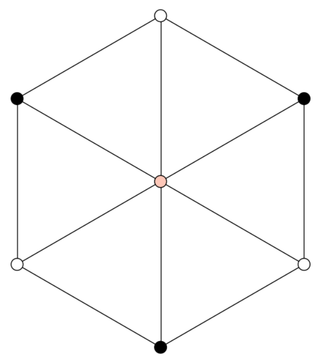

Figure 2.1: 3-Colouring of a wheel graph

For us it will be more convenient to define it in terms of homomorphisms.

Definition (Classical homomorphism)**.** *Homomorphism* from a graph X to graph Y is a function $f : V(X) \to V(Y)$ such that whenever x and x' are adjacent (denoted by $x \sim x'$) in X, it holds that $f(x) \sim f(x')$ in Y as well.

This theorem will serve as our definition of a chromatic number.

2.1.1 Theorem. *[13] The chromatic number of the graph X is the least integer r such that there is a homomorphism from X to K_r.*

Proof. Suppose that the chromatic number of a graph is r. Vertices of K_r correspond to colours $1, ..., r$. Now, define a homomorphism from

$$\begin{aligned} h &: X \to K_r \\ h(v) &\mapsto \text{ colour of } v \end{aligned}$$

Now, if two vertices are adjacent in X, they will have different colours, and thus will map to adjacent vertices of K_r. If they are of the same colour, they are not adjacent and are mapped to the same vertex in K_r. Since K_r is loopless, h is a homomorphism. The choice of r was minimum, so the statement follows.

On the other hand, if there is a homomorphism $h : X \to K_r$ then for each $i \in K_r$ each $h^{-1}(i)$ corresponds to a colour class, consisting of nonadjacent vertices. Thus,

$$\text{colour}(v) = i \text{ if } i \in h^{-1}(i)$$

is a valid r-colouring. □

Coclique number, also referred as independence number, is the size of a maximal subset of vertices of a graph such that no two are adjacent. It would be called the clique number in the complement of the graph.

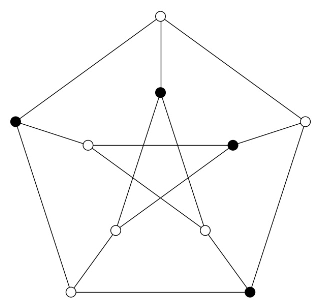

Figure 2.2: 4-coclique in the Petersen graph

As for the chromatic number, we will give a general definition for the independence number of the graph and then the one in terms of homomorphisms, which will be more useful to us.

There are multiple connections between independent sets and colourings. For example, in a proper colouring of X, colour classes (vertices of the same colour) are cocliques. Additionally, $\chi(X) \geq \alpha(\overline{X}) = \omega(X)$ There is an analogous theorem for quantum independence number in terms of homomorphisms.

2.1.2 Theorem. *[13] The coclique number of the graph X is the largest integer s such that there is a homomorphism from K_s to $\overline{X}$.*

Proof. Suppose, S is a maximal independent set in X with the size s. In the complement $\overline{X}$, the set $S = \{s_1, ..., s_s\}$ will correspond to a K_s subgraph. Now, define a homomorphism from

$$h : K_s \to \overline{X}$$

$$h(v) \mapsto s_v.$$

Now, this is an inclusion homomorphism.

On the other hand, if s is the largest integer such that there is a homomorphism $h : K_s \to \overline{X}$, then there is a K_s clique subgraph in $\overline{X}$, corresponding to an s-coclique in X. □

2.2 Quantum definitions

At first the definition of a quantum homomorphism may look totally unrelated to the classical one.

Definition. [21] There exists a *quantum homomorphism* from X to Y if and only if there exist a $|V(X)| \times |V(Y)|$ matrix E with projections $E^{(x,y)}$ in the (x, y)-entry such that

- $\sum_{y \in V(Y)} E^{(x,y)} = I \quad$ for all $x \in V(X)$
- $E^{(x,y)} E^{(x',y')} = 0$ if $(x = x'$ and $y \neq y')$ or $(x \sim x'$ and $y \nsim y')$

If we consider projections to be 1×1 matrices which get values either 0 or 1, then this definition easily reduces to the classical homomorphism. Suppose, $h : X \to Y$ is an (X, Y)-homomorphism. Let

$$E^{(x,y)} = \begin{cases} 1 \text{ if } h(x) = y, \\ 0 \text{ otherwise }. \end{cases}$$

One can check that this is a valid quantum homomorphism.

When the projections of interest are not one-dimensional, in [26] Roberson demonstrates a way to translate the question about quantum homomorphisms into a language of the better studied classical homomorphisms. For this a concept of measurement graph is useful.

Definition (Measurement graph)**.** [26]

For us a *projective measurement*, on a set S is a set of projections in $\mathbb{C}^{d \times d}$, that sum to identity (implying they are pairwise orthogonal) and are indexed by the elements of the set S.

For a finite graph Y and $d \in \mathbb{N}$, define the *measurement graph* $M(Y, d)$ to be the graph whose vertices are projective measurements on the set $V(Y)$. Two vertices $\{P_y\}_{y \in V(Y)}$ and $\{Q_y\}_{y \in V(Y)}$ are adjacent if $P_y Q_{y'} = 0$ for all $y \nsim y'$.

2.2.1 Theorem. *[26] If X and Y are graphs, then $X \xrightarrow{q} Y$ if and only if $X \to M(Y, d)$ for some $d \in \mathbb{N}$.*

Proof. Suppose, $f : X \to M(Y, d)$. Let $f(x) = E^x$. Let $E^{(x,y)} = E^x_y$. It follows from the definition of the measurement graph that projections $E^{(x,y)}$ satisfy the conditions in the definition of the measurement graph.

On the other hand, if $X \xrightarrow{q} Y$, then there exist projections $E^{(x,y)}$ satisfying the conditions in the definition of the quantum homomorphism. Let

$$\begin{aligned} f : V(X) &\to V(M(Y, d)) \\ x &\mapsto E^x = \{E^{(x,y)}\}_{y \in V(Y)} \end{aligned}$$

Then if $x \sim x'$, we have that $E^{(x,y)}E^{(x',y')} = 0$ if y is not adjacent to y' and and f is indeed a homomorphism. □

Now we are going to define χ_q and α_q in terms of projections.

2.2.1 Quantum chromatic number

In the literature χ_q is defined analogously to χ through, now a quantum, homomorphism. Thus, $\chi_q(X)$ is the smallest s such that there is a quantum homomorphism from X into K_s. In other words, there are projections $P^{(u,i)}$ for $u \in V(X)$ and $i = 1, ..., s$ such that

- $\sum_{i=1,\dots,s} P^{(u,i)} = I_d$ for all $u \in V(X)$ and
- $P^{(u,i)}P^{(v,j)} = 0$ if $(i = j$ and $u \neq v)$ or $(i \sim j$ and $u \nsim v)$

We can rewrite it in a more convenient way.

Definition. For a graph X, the *quantum chromatic number* $\chi_q(X)$ is the minimum integer s for which there exist a $|V(X)| \times s$ block matrix P such that $P^{(u,i)} \in \mathbb{C}^{d \times d}$ is a projection, and its entries satisfy the following conditions:

- $\sum_{i \in 1,\dots,s} P^{(u,i)} = I_d$ for all $u \in V(X)$ and
- $\langle P^{(u,i)}, P^{(v,i)} \rangle = 0$ for all $uv \in E(X)$ and $i = 1, ..., s$

We will often concentrate on the entries $\{P^{(u,i)}\}_{u \in V(X), i \in [s]}$ themselves, without recalling the matrix explicitly.

As a careful reader notices, d is not fixed in the definition. This pushes various definitions with a concrete d, such as $\chi_{\mathbf{q}}^{(\mathbf{1})}$, a *rank one quantum chromatic number*, where $d = 1$. If we have the matrix Q for the rank-1 quantum chromatic number, it also satisfies the conditions for χ_q. It means that $\chi_q \leq \chi_q^{(1)}$ for all graphs.

A lot of graphs studied in this thesis will be *orthogonality graphs* for some set of vectors from some Hilbert space $\mathbb{H}$. Vertices of such graphs are the chosen vectors and two vertices are made adjacent only if the corresponding vectors are orthogonal. The dimension of $\mathbb{H}$ is the *dimension* of this *orthogonal representation*.

On the other hand, a graph G on n vertices has *orthogonal representation* in some Hilbert space $\mathbb{H}$ if there is a homomorphism from G into an orthogonality graph of a subset of vectors in $\mathbb{H}$.

Example. For example, vectors $(1,0,0), (0,1,0)$ and $(0,0,1)$ determine an orthogonal representation of K_3 in $\mathbb{R}^3$.

Some graphs with the known quantum chromatic number rely on the dimension of vectors the orthogonal representation of the graph to determine the quantum chromatic number. Therefore, it can be interesting to know the lowest such dimension, also known as the *orthogonal rank*, ξ of the graph.

Here we present a couple of related theorems.

2.2.2 Theorem. *[7]* $\xi(X) \leq \chi_q^{(1)}(X)$.

Proof. Suppose, X is a graph with $\chi_q^{(1)}(X) = k$, obtained by rank-1 $d \times d$ projections $\{P^{(u,i)}\}_{u \in V(X), i \in [k]}$. Observe, that since projections are rank-1, they can be written as $P^{(u,i)} = u_i u_i^*$ for any $u \in V(X), i \in [k]$. Now, we must have d rank-1 projections adding up to I_d, which means that $\chi_q^{(1)}(X) = d$.

Now, we from the definition of the quantum chromatic number, it follows that for every u adjacent to v,

$$\langle P^{(u,1)} P^{(v,1)} \rangle = \langle u_1 u_1^*, v_1 v_1^* \rangle = 0$$

which happens if and only if

$$\langle u_1, v_1 \rangle = 0.$$

To obtain the orthogonality representation of the graph, only consider the projections from the quantum coclique matrix in the column 1, i.e.

$$\{P^{(u,1)} = u_1 u_1^*\}_{u \in V(G)}$$

and define a homomorphism into the orthogonality graph of the vectors $\{u_1\}_{u \in V(G)}$:

$$u \mapsto u_1,$$

which is a valid orthogonal representation of G. Hence, $\xi(X) \leq d \leq \chi_q^{(1)}(X)$. □

2.2.3 Theorem. *[7] If a graph X has a real orthogonal representation in dimension 3 or 4, then $\chi_q(X) \leq 4$. Similarly, if X has a real orthogonal representation in dimension 8, then $\chi_q(X) \leq 8$.*

Remark. *Cameron et al in [7] only prove the theorem for dimension 4. They claim that the analogous proof works for dimension 8, without providing the proof. We verified the construction in dimension 8.*

The proof of this theorem is taken from [20].

Proof. Clearly, a 3-dimensional orthogonal representation can be easily lifted to a 4-dimensional one by adding a 0 last coordinate to each of the vectors, so it suffices to consider the 4-dimensional case only.

Cameron et al. in [7] provide a method to construct a quantum 4-colouring relying on the 4-dimensional orthogonal representation.

Suppose $\mathbf{r} = (r_0, r_1, r_2, r_3)^T \in \mathbb{R}^4$ is a unit vector (for us later will be coming from an orthogonal representation). We will describe how to construct a full orthonormal basis from it. If we do that, then the projections on each of the basis vectors will give us projections that sum to identity, and will be a good candidate for projections v_i for a quantum colouring of a vertex $v \in G$.

Thus, associate to any vector $\mathbf{r} \in \mathbb{R}^4$ a quaternion

$$q(\mathbf{r}) = r_0 g_0 + r_1 g_1 + r_2 g_2 + r_3 g_3,$$

where $g_0 = 1, g_1 = \mathbf{i}, g_2 = \mathbf{j}, g_3 = \mathbf{k}$. The $g_{0,1,2,3}$ notation is easier to refer to quaternions, because of the imaginary unit i. Thus, we have that $g_m^2 = -1$ for $m = 1, 2, 3$ and for distinct $i, j \in \{1, 2, 3\}$, we have $g_i g_j = \pm g_k$ for some $k \in \{1, 2, 3\} \setminus \{i, j\}$. Similar rules also hold for octonions. For convenience, we also include the multiplication table here:

	1	i	j	k
1	1	i	j	k
i	i	-1	k	-j
j	j	-k	-1	i
k	k	j	-i	-1

Figure 2.3: Octonions multiplication table, [3]

Now, for all $i \in \{0, 1, 2, 3\}$ define $\mathbf{r}_i \in \mathbb{R}^4$ to be the vectors such that $q(\mathbf{r}_i) = g_i q(\mathbf{r})$. For example, for $\mathbf{r}^0$ we want a vector such that

$$q(\mathbf{r}_0) = g_0 q(\mathbf{r}) = r_0 g_0^2 + r_1 g_0 g_1 + r_2 g_0 g_2 + r_3 g_0 g_3.$$

However, since $g_0 = 1$, we get that

$$q(\mathbf{r}_0) = r_0 g_0 + r_1 g_1 + r_2 g_2 + r_3 g_3 = q(\mathbf{r}),$$

so $\mathbf{r}_0 = \mathbf{r}$. Another example is $\mathbf{r}^1$. We are looking for a vector such that

$$q(\mathbf{r}_1) = g_1 q(r) = r_0 g_1 g_0 + r_1 g_1 g_1 + r_2 g_1 g_2 + r_3 g_1 g_3 = r_0 g_1 - r_1 g_0 + r_2 g_3 - r_3 g_2,$$

where the last equality comes from the property of quaternions and yields a vector

$$q(\mathbf{r}_1) = (-r_1, r_0, -r_3, r_2,)^T$$

when written in the quaternion basis. In a similar manner we could write the remaining vectors obtained from $\mathbf{r}$ in a matrix form, i.e. $(\mathbf{r}_0, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3)^T =$

$$\begin{bmatrix} r_0 & -r_1 & -r_2 & -r_3 \\ r_1 & r_0 & r_3 & -r_2 \\ r_2 & -r_3 & r_0 & r_1 \\ r_3 & r_2 & -r_1 & r_0 \end{bmatrix}$$

Here we will show that $\{\mathbf{r}_0, \mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3\}$ form an orthonormal basis. The i^{th} entry in the j^{th} column corresponds to the coefficient in front of r_j in the quaternions basis. We can just double check by multiplying the vectors out in quaternions basis that they are orthogonal.

There is a more systematic way too. One can see the pattern after we show why $\mathbf{r}_1, \mathbf{r}^2, \mathbf{r}^3$ are orthogonal to $\mathbf{r}^0 = \mathbf{r}$. First, observe that left-multiplying $q(r)$ by g_i swaps the coefficients g_0 and g_i with an opposite sign (as in the matrix the new g_0's are $-r_1, -r_2$ and $-r_3$. So the new coefficients for g_0 and g_i contribute nothing to the inner product (e.g. for $\mathbf{r}_0$ and $\mathbf{r}_2$, we get $-r_0r_2 + r_2r_0$ for the 0^{th} and 2^{nd} coordinates.)

The same is true of the remaining coordinates. When calculating the expression for $\langle \mathbf{r}_0, \mathbf{r}_m \rangle$ we will face the summation $g_1g_ig_1 + g_jg_ig_j$, where in general $i \neq 0, j, 1$. By properties of quaternions, $g_1g_ig_1 = g_jg_1$ and $g_jg_ig_j = g_1g_j = -g_jg_1$. In other words, those also contribute 0 to the inner product, so each of $\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3$ is orthogonal to $\mathbf{r}_0$. Similar arguments show that they are pairwise orthogonal as well.

Second, recall that $\mathbf{r}$ was a unit vector. Since multiplying by g_i just permutes the elements of the group and they all have the same norm, $q(\mathbf{r})$ is a unit vector too. Now, we obtained $\mathbf{r}_i$ by changing signs and rearranging entries of $\mathbf{r}$, hence, we did not change its norm. We see that all $\mathbf{r}_i$ are unit vectors.

Now, suppose a graph X has an orthogonal representation ϕ in dimension 4. Using the above construction and letting $\phi(v) = \mathbf{r}$, we can construct orthonormal basis $\{\phi(v)_0, \phi(v)_1, \phi(v)_2, \phi(v)_3\}$ as above. As mentioned in the beginning, we can let v_i be a projection onto the vector $\phi(v)_i$. Since $\phi(v)_i$'s come from an orthonormal basis, $\sum_i v_i = I_4$ and $\langle v_i, v_j \rangle = 0$ if and only if $\langle \phi(v)_i, \phi(v)_j \rangle = 0$, which holds from again $\phi(v)_i$'s forming a basis.

We have just shown how given a 4-dimensional real orthogonal representation, we can construct a quantum 4-colouring. □

There is a similar construction for dimension 8 orthogonal representation with help of octonions. Since we have not found the proof written out in the literature, we provide it here.

Proof. We verify that all of the above steps work in dimension 8 as well. Consider a unit vector $\mathbf{r} = (r_0, ..., r_7)^T \in \mathbb{R}^8$. As before, we will try to construct an orthonormal basis for $\mathbb{R}^8$ from it. With every such vector $\mathbf{r}$, Associate an octonion

$$p(\mathbf{r}) = r_0e_0 + r_1e_1 + ... + r_7e_7,$$

where $e_0, ..., e_7$ are octonions. Now for all $i = 0, ..., 7$, let $\mathbf{r}^i \in \mathbb{R}^8$ be the vector such that $p(\mathbf{r}^i) = e_ip(\mathbf{r})$. For example, $\mathbf{r}^0 = \mathbf{r}$. As a slightly advanced example,

$$\begin{aligned} q(\mathbf{r}^1) &= e_1(r_0e_0 + r_1e_1 + ... + r_7e_7) \\ &= -r_1e_0 + r_0e_1 - r_3e_2 + r_2e_4 - r_5e_4 + r_4e_5 + r_7e_6 - r_6r_7, \end{aligned}$$

Where the last equality is using the octonions multiplication rules.

$$\mathbf{r}^i = (-r_1, r_0, -r_3, r_2, -r_5, r_4, r_7, -r_6)^T.$$

Placing the column vectors $\mathbf{r}^0, ..., \mathbf{r}^7$ results in the following matrix.

$$\begin{bmatrix} r_0 & -r_1 & -r_2 & -r_3 & -r_4 & -r_5 & -r_6 & -r_7 \\ r_1 & r_0 & r_3 & -r_2 & r_5 & -r_4 & -r_7 & r_6 \\ r_2 & -r_3 & r_0 & r_1 & r_6 & r_7 & -r_4 & -r_5 \\ r_3 & r_2 & -r_1 & r_0 & r_7 & -r_6 & r_5 & -r_1 \\ r_4 & -r_5 & -r_6 & -r_7 & r_0 & r_1 & r_2 & r_3 \\ r_5 & r_4 & -r_7 & r_6 & -r_1 & r_0 & -r_3 & r_2 \\ r_6 & r_7 & r_4 & -r_5 & -r_2 & r_3 & r_0 & -r_1 \\ r_7 & -r_6 & r_5 & r_4 & -r_3 & -r_2 & r_1 & r_0 \end{bmatrix}$$

We will show that its columns are pairwise orthogonal, and thus, $\mathbf{r}^0, ..., \mathbf{r}^7$ form a basis. The reasoning is very similar to the one in the 4-dimensional case. Left multiplying $\mathbf{r}$ by e_i swaps r_{2j} and r_{2j+1} for $j = 0, 1, 2, 3$ with making one of the elements negative. Recall that all the coefficients $r_0, ..., r_7$ are real numbers, so the vector $\mathbf{r}^0 = \mathbf{r}$ is orthogonal to any $\mathbf{r}^i, i = 1, ..., 7$, in $\mathbb{R}^8$.

Looking at the multiplication table of octonions (provided below), one can notice that for any pair of e_i and e_j there are 4 pairs (k, m) of elements e_k and e_m such that, up to inverting all the signs:

$$\begin{aligned} e_ie_\alpha &= e_k \\ e_je_\alpha &= e_m \end{aligned}$$

and

$$\begin{aligned} e_ie_\beta &= e_m \\ e_je_\beta &= -e_k \end{aligned}$$

		e_j							
	$e_i e_j$	e_0	e_1	e_2	e_3	e_4	e_5	e_6	e_7
e_i	e_0	e_0	e_1	e_2	e_3	e_4	e_5	e_6	e_7
	e_1	e_1	$-e_0$	e_3	$-e_2$	e_5	$-e_4$	$-e_7$	e_6
	e_2	e_2	$-e_3$	$-e_0$	e_1	e_6	e_7	$-e_4$	$-e_5$
	e_3	e_3	e_2	$-e_1$	$-e_0$	e_7	$-e_6$	e_5	$-e_4$
	e_4	e_4	$-e_5$	$-e_6$	$-e_7$	$-e_0$	e_1	e_2	e_3
	e_5	e_5	e_4	$-e_7$	e_6	$-e_1$	$-e_0$	$-e_3$	e_2
	e_6	e_6	e_7	e_4	$-e_5$	$-e_2$	e_3	$-e_0$	$-e_1$
	e_7	e_7	$-e_6$	e_5	e_4	$-e_3$	$-e_2$	e_1	$-e_0$

Figure 2.4: Octonions multiplication table, [2]

Thus, when taking inner products of columns corresponding to the vectors $\mathbf{r}^i$ and $\mathbf{r}^j$, the summands will consist of pairs of the type $e_k e_m - e_m e_k = 0$, making any two such columns orthogonal.

Now, if we have an 8-dimensional orthogonal representation, we can construct a quantum 8-colouring as follows. For a vertex v with a vector $\mathbf{r}$, assign projections $\{\mathbf{r}^0(\mathbf{r}^0)^T, ..., \mathbf{r}^7(\mathbf{r}^7)^T\}$. They sum to identity, as rank-1 projections built from a basis. The orthogonality conditions still hold as the orthogonality conditions hold for the underlying vectors. $\square$

2.2.2 Quantum independence number

Analogously, define α_q as the largest t such that there is a quantum homomorphism from $K_t \xrightarrow{q} \overline{X}$. This corresponds to a quantum clique number of the complement $\omega_q(\overline{X})$. In this case, the Definition 2.2 guarantees the existence of projections $E^{(x,y)}$ such that

- $\sum_{x\in V(X)} E^{(x,i)} = I_d \quad \forall i \in V(K_t) \qquad (1)$
- $E^{(x,i)}E^{(x',j)} = 0$ if ($i = j$ and $x \neq x'$) or ($i \sim j$ and $x \nsim x'$) $\qquad (2)$

By labelling vertices of K_t as $\{1, ..., t\}$, noting that $i \sim j$ in K_t if and only if $i \neq j \in [t]$, and observing that $x \nsim x$ covers the case that $x = x'$, we rewrite the definition in the more compact form.

Definition. For a graph X, *quantum coclique number* $\alpha_q(X)$ is the maximum integer t for which there exist a $|V(X)| \times t$ block matrix P with $P^{(u,i)} \in \mathbb{C}^{d\times d}$, a projection such that

- $\sum_{v\in V(X)} P^{(u,i)} = I_d$ for all $i = 1, ..., t$
- $P^{(u,i)}P^{(v,j)} = 0$ for any $u \sim v$ for all $i, j = 1, ..., t$
- $P^{(u,i)}P^{(u,j)} = 0$ for any $i \neq j$ for all $i, j = 1, ..., t$ and $u \in V(X)$

As in the case with the quantum chromatic number, we will concentrate on the entries $\{P^(u, i)\}_{u\in V(X), i\in[t]}$ themselves, without recalling the matrix explicitly.

2.3 Linear Algebra

At this point it is clear that we will be dealing a lot with projections, so it helps to recall some of their properties. For $d \times d$ projections P and Q we recall some general facts:

- $PQ = 0$ if and only if $\langle P, Q\rangle = 0$
- Since $P^2 = P$, the eigenvalues of P are 0 and 1.
- Therefore, P is positive semidefinite.
- If projections $\{P_i\}_i = 1, ..., k$, are mutually orthogonal, then

$$\operatorname{rk} \sum_i P_i = \sum_i \operatorname{rk} P_i.$$

There is another more elaborate result about the sum of projections that sum to identity.

2.3.1 Theorem. *[9] Suppose $A_i, i = 1, ..., m$ are $n \times n$ complex matrices and let n_i denote the rank of A_i. Then if $\sum_{i=1}^m A_i = I_n$ the following are equivalent:*

1. $A_i^2 = A_i$
2. $\sum_i n_i = n$
3. $A_i A_j = 0$ *for all* $i, j = 1, ..., m$ *and* $i \neq j$, $\square$

2.4 Analogues of classical results

There are quite a few similarities between the quantum and classical parameters.

2.4.1 Lemma. *If* $X \xrightarrow{q} Y$, *then* $\chi_q(X) \leq \chi_q(Y)$.

Proof. Consider a quantum homomorphism $Y \xrightarrow{q} K_k$. We can compose quantum homomorphisms to obtain $X \xrightarrow{q} Y \xrightarrow{q} K_k$. Since we are looking for the smallest n such that there is a quantum homomorphism from X to K_n, we conclude that $\chi_q(X) \leq \chi_q(Y)$. $\square$

To the best of our knowledge the rest of this subsection provides some new results.

2.4.2 Lemma. *Consider a graph* X. *Let* Y *be obtained by adding an apex vertex* v *to* X, *then* $\alpha_q(X) = \alpha_q(Y)$.

Proof. First, if projections $\{P^{(u,i)}\}_{i\in[t]}^{u\in X}$ determine a t-quantum coclique in X, then we can just assign t zero projections to v. Hence, $\alpha_q(Y) \geq \alpha_q(X)$.

Now, suppose

$$\{Q^{(u,i)}\}_{i\in[k]}^{u\in Y}$$

determine a k-quantum coclique in Y. We will create a quantum k-coclique in X. First, delete the vertex v from Y and choose an arbitrary vertex $u \in X$. Update projections of u from $Q^{(u,i)}$ to

$$R^{(u,i)} = Q^{(u,i)} + Q^{(v,i)}.$$

Leave the remaining projections unchanged:

$$R^{(x,i)} = Q^{(x,i)} \text{ for } x \neq u.$$

We will prove that $\{R^{(x,i)}\}_{x\in X}^{i\in[t]}$ determine a k-quantum coclique in X.

We have that

$$R^{(u,i)}R^{(u,j)} = (Q^{(u,i)} + Q^{(v,i)})(Q^{(u,j)} + Q^{(v,j)}) = 0$$

if $i \neq j$, since u and v are adjacent in Y. Similarly, for $x \neq u, i \neq j$

$$R^{(x,i)}R^{(x,j)} = Q^{(x,i)}Q^{(x,j)} = 0.$$

Now,

$$\sum_{x \in X} R_{(x,i)} = \sum_{x \in Y} Q_{(x,i)} = I.$$

Moreover, if $y \neq u$ and $i \neq j$ and $x \sim y$

$$R_{(x,i)}R_{(y,j)} = Q_{(x,i)}Q_{(y,j)} = 0.$$

Finally, if $x \sim u$ and $i \neq j$, then

$$R^{(x,i)}R^{(u,j)} = Q^{(x,i)}(Q^{(u,j)} + Q^{(v,j)}) = 0),$$

because $x \sim v$ in Y for all $x \in X$. Therefore, $\alpha_q(X) \geq \alpha_q(Y)$. The statement follows. □

Using Lovász's ϑ, we can prove that Paley(13) exhibits no separation between the classical and quantum independence numbers. We are going to define Paley(13) below, while ϑ is just a bound aiding our calculations. The curious reader is welcome to explore more about this parameter in the Section 6.3.

Definition. [13] For a prime power $q \equiv 1 \bmod 4$, Paley graph $P(q)$ has as vertex set the elements of the finite field $GF(q)$, with two vertices being adjacent if and only if their difference is a nonzero square in $GF(q)$.

It is well-known, that for any $q \equiv 1 \bmod 4$, a Paley graph $P(q)$ is isomorphic to its complement. [17]. They are also known to be vertex-transitive [13]. A graph G is *vertex-transitive* if for any two vertices u and v there is a homomorphism $h : G \to G$ from the graph to itself mapping u to v.

2.4.3 Theorem ([17]). *If G has n vertices, is isomorphic to its complement and has a vertex-transitive automorphism group, then*

$$\vartheta(G) = \sqrt{n}.$$ □

This theorem can help establish quantum independence number when other bounds may be not tight enough, as illustrated in the example below.

Example. $\alpha(P(13)) = \alpha_q(P(13)) = 3$.

Proof. From the above theorem, we get that $\vartheta(P(13)) = \sqrt{13} < 4$. Using the bound from [5]:

$$3 = \alpha(P(13)) \leq \alpha_q(P(13)) \leq 3. \qquad \square$$

2.4.4 Lemma. *Suppose, G is a graph on n vertices, then $\alpha(G) = 2$ if and only if $\alpha_q(G) = 2$.*

Proof. For the easier only if direction, suppose that $\alpha_q(G) = 2$. Since

$$\alpha(G) \leq \alpha_q(G),$$

we can only have $\alpha = 1$ or $\alpha = 2$. The only graph with $\alpha = 1$ on n vertices is a complete graph K_n. However, the so called inertia bound on the classical and quantum coclique from [29] says that

$$\alpha(K_n) \leq \alpha_q(K_n) \leq \min\{n_0(K_n) + n_+(G), n_0(K_n) + n_-(K_n)\},$$

where $n_0(K_n)$ is the number of zero eigenvalues of the adjacency matrix of the graph G, the $n_+(K_n)$ is the number of positive eigenvalues of the adjacency matrix of the graph and $n_-(K_n)$ is the number of negative eigenvalues of the adjacency matrix of the graph. One can see that $n_0(K_n) + n_+(K_n) = 1$ for any complete graph, and thus $\alpha_q(K_n) = 1$ as well. We conclude that if $\alpha_q(G) = 2$, then $\alpha(G) = 2$.

Now we will prove the the if direction.

Claim: If a graph G has a quantum t coclique assignment, it has a quantum $t-1$ coclique assignment.

Proof: Suppose $\alpha_q(G) = t$, given by projections $\{P^{(u,i)}\}_{i\in[t]}^{u\in V(G)}$. Then we can get projections $\{Q^{(u,i)}\}_{i\in[t-1]}^{u\in V(G)}$ satisfying the quantum coclique requirements as follows:

$$P^{(u,i)} = \begin{cases} P^{(u,i)} & \text{if } i < t-1, \\ \frac{1}{2}(P^{(u,i)} + P^{(u,i+1)}) & \text{if } i = t-1. \end{cases}$$

One can check that this is a valid $t-1$ quantum coclique projection assignment. ■

Thus, without loss of generality, towards contradiction, assume that there is a 3-quantum coclique assignment $\{P^{(u,i)}\}_{i\in 3}^{u\in V(G)}$. From the quantum coclique definition, for each index (column), we get the column sums:

$$\begin{aligned} P^{(u_1,1)} + ... + P^{(u_n,1)} &= I \\ P^{(u_1,2)} + ... + P^{(u_n,2)} &= I \qquad (*) \\ P^{(u_1,3)} + ... + P^{(u_n,3)} &= I. \end{aligned}$$

Now, choose an arbitrary vertex v, and multiply each of these expressions by $P^{(v,i)}$ for $i = 1, 2, 3$. We obtain that for each $i \neq j$ and $j \in \{1, 2, 3\}$:

$$\begin{aligned} P^{(v,1)}\big(P^{(w_1,j)} + ... + P^{(w_s,j)}\big) &= P^{(v,1)} \\ P^{(v,2)}\big(P^{(w_1,j)} + ... + P^{(w_s,j)}\big) &= P^{(v,2)} \\ P^{(v,3)}\big(P^{(w_1,j)} + ... + P^{(w_s,j)}\big) &= P^{(v,3)}. \end{aligned}$$

Where $W = \{w_1, ..., w_s\}, s \leq n$ are the non-neighbours of v. Moreover, since $\alpha(G) = 2$, every set of 3 vertices of G has at least two vertices with an edge between them. For the set of any two non-neighbours of v and v that looks like $\{w_a, w_b, v\}$, we have to have that there is an edge $w_a w_b$. It follows, that W form a clique in G. Now, multiply each expression

$$P^{(v,i)}\big(P^{(w_1,j)} + ... + P^{(w_s,j)}\big) = P^{(v,i)}$$

for $i \neq j$ and all $i = 1, 2, 3$ on the right by some $P^{(w_c,k)}$, such that in a such expression $k \neq i, k \neq j, w_c \in W$ [notice that it is possible to choose such k, because the assumption is $\alpha_q \geq 3$]. Since W is a clique, any $P^{(w_a,j)}P^{(w_c,k)} = 0$. In this way, we get that $P^{(v,i)}P^{(w_c,k)} = 0$ with the condition that v and w_c are not adjacent and $i \neq k$.

Hence, when multiplying all three equations from $(*)$ together, we will be left with

$$\sum_{i,j,k=1,...,|V(G)|} P^{(u_i,1)}P^{(u_j,2)}P^{(u_k,3)} = 0 \neq I,$$

because $P^{(u_i,a)}P^{(u_j,b)} = 0$ if $u_i \sim u_j$ by definition of quantum coclique, and $P^{(u_i,a)}P^{(u_j,b)} = 0$ if $u_i \nsim u_j$ and $a \neq b$ from above. The desired contradiction is achieved. □

2.5 Quantum measurements

To smoothly transition into the chapter on Kochen-Specker theorem, we present some of the quantum-mechanical formalism.

We will encounter measurements and quantum states a lot in basic context. Therefore, here we provide some background on these topics. For us, a quantum state will be a norm one vector in $\mathbb{C}^d$. In quantum mechanics, there is no determined state of a quantum system in a given moment, but instead the corresponding vector provides probability of an outcome of any possible measurement. For example, consider a state

$$\psi = a_1 e_1 + a_2 e_2 + a_3 e_3 + a_4 e_4,$$

where $e_1, ..., e_4$ form an orthonormal basis for $\mathbb{C}^4$. Quantum mechanics states that if we perform a measurement in the standard basis, we will have a probability

$$p_i = |\langle v, e_i \rangle|^2$$

of measuring the e_i's basis vector. As such, the probability of an outcome being $|00\rangle$ is $|a|^2$. We could also perform a measurement in a different orthogonal basis. For knowing the probabilities of the outcomes, we would need to rewrite our state vector in the new basis, and take the squared values of the amplitudes [1].

Peres [22] defines a quantum measurement to be a quantum test with outcomes labelled by real numbers. There is a Mathematical way to think about it. The measurement in quantum mechanics is a set of matrices $\{M_i\}_i$, with indices referring to those real outcomes satisfying

$$\sum_i M_i^* M_i = I.$$

. If our system is in the state ψ, then the probability of outcome i is defined to be

$$\psi^* M_i^* M_i \psi.$$

We see that the sum-to-identity requirement guarantees that the total probability over all outcomes is one.

Finally, part of quantum reality is a collapse of the state to the post-measurement state

$$\frac{M_i|\psi\rangle}{\sqrt{\psi^* M_i^* M_i \psi}},$$

which will have to be an eigenvector of the observable.

For our purposes, we just need *projective measurements* where M_i's are projections. We have that a projective measurement is a set $\{P_i\}_i$ of pairwise orthogonal projections in $\mathbb{C}^{d\times d}$ summing to I_d.

In the example above, we could choose a $\{P_i = e_i e_i^*\}_i$. As expected, the probability of the outcome i would be

$$\psi^* P_i \psi = a_i a_i^* = \|a_i\|^2.$$

After this measurement, the state will become

$$\frac{a_i e_i}{\|a_i\|},$$

which is just e_i up to the phase. [1]

Chapter 3

Background on the Kochen-Specker theorem

3.1 Kochen-Specker theorem as a consequence of Gleason's theorem

Gleason's theorem and the Kochen-Specker theorem are two fundamental results in Quantum Physics.

Before stating the theorems, we first start with definitions. A lot of material here is taken from [24]. We use the simplified version of the Gleason's frame function. A real function f defined over the unit vectors in $\mathbb{R}^n$ is called a *frame function* if:

1. For all unit vectors x, we have $f(x) \geq 0$.

2. There is a constant C_f such that for every orthonormal basis $x_1, ..., x_n$ in $\mathbb{R}^n$, we have $\sum_{k=1}^{n} f(x_k) = C_f$.

The number C_f is called the weight of the frame function. If we restrict values of the frame function to weight $C_f = 1$ and only allow the function f to have values 0 and 1, then we obtain what is known in literature as the marking function. *A marking function* on $S \subseteq \mathbb{R}^n$ is a function $f : S \to \{0, 1\}$ such that for all orthonormal bases $B \subseteq S$ we have $\sum_{u \in B} f(u) = 1$.

Now, we are ready to state Gleason's theorem.

3.1.1 Theorem (Gleason's theorem)**.** *Let f be a non-negative frame function on a real (or complex) separable Hilbert space $\mathbb{H}$ of dimension $d \geq 3$.*

Then there is a self-adjoint, positive semidefinite operator W on $\mathbb{H}$ such that $f(x) = x^T W x$.

Gleason has proved that whenever a frame function exists, it will have to be continuous. The proof can be found in [24]. Using Gleason's theorem it is possible to prove that the orthogonality graph of a unit sphere in $\mathbb{R}^3$ cannot be three coloured. Indeed, if we have a three-colouring, define a function $g : S^3 \to \{0, 1\}$ such that

$$g(v) = \begin{cases} 1 \text{ if } v \text{ is coloured colour } 1 \\ 0 \text{ otherwise.} \end{cases}$$

Such g satisfies the definition of the frame function (and marking function), since its evaluation sums to 1 on each maximal 3-clique. However, g is not continuous. By compactness it follows that there is a finite subset of vectors in $\mathbb{R}^3$, such that their orthogonality graph cannot be 3-coloured, in other words, on which there is no marking function. Kochen-Specker theorem finds such set of vectors explicitly [11].

3.1.2 Theorem (Kochen-Specker)**.** *[22] There is a finite set M of projections in $\mathbb{C}^{d \times d}$, such that there is no marking function $f : M \to \{0, 1\}$ satisfying*

$$\sum_{P \in S \subset M} f(P) = 1.$$

Observe, that the Kochen-Specker theorem is stated using rank-1 projections $\{P\}_{P \in M}$, not vectors. However, we can associate each rank-1 projection P with its corresponding vector x such that $P = xx^T$.

In their original proof, Kochen and Specker come up with the set of vectors which has no marking function. Therefore, sets of vectors in $\mathbb{C}^d$ for which there is no marking function became known as *Kochen-Specker seta.*

There have been a number of proofs of the Kochen-Specker theorem for dimension $d \geq 4$, and they are shorter and easier to understand. The proofs by Cabello et al. [6] and [15] differ only in the number of vectors: 18 and 20 respectively. The proofs demonstrate there is no marking function using equations. We will present a proof here which generalises one approach to prove the Kochen-Specker theorem in $d \geq 4$. For example, we will take a brief look at Kernaghan's proof.

Proof. [15] In the proof we use non-unit vectors for visual convenience, but they can be normalised without influencing the proof. Here is the system of equations that Kernaghan proves is inconsistent.

$$
\begin{aligned}
1 &= f(1,0,0,0) + f(0,1,0,0) + f(0,0,1,0) + f(0,0,0,1)\\
1 &= f(1,0,0,0) + f(0,1,0,0) + f(0,0,1,1) + f(0,0,1,-1)\\
1 &= f(1,0,0,0) + f(0,0,1,0) + f(0,1,0,1) + f(0,1,0,-1)\\
1 &= f(1,0,0,0) + f(0,0,0,1) + f(0,1,1,0) + f(0,1,-1,0)\\
1 &= f(-1,1,1,1) + f(1,-1,1,1) + f(1,1,-1,1) + f(1,1,1,-1)\\
1 &= f(-1,1,1,1) + f(1,1,-1,1) + f(1,0,1,0) + f(0,1,0,-1)\\
1 &= f(1,-1,1,1) + f(1,1,-1,1) + f(0,1,1,0) + f(1,0,0,-1)\\
1 &= f(1,1,-1,1) + f(1,1,1,-1) + f(0,0,1,1) + f(1,-1,0,0)\\
1 &= f(0,1,-1,0) + f(1,0,0,-1) + f(1,1,1,1) + f(1,-1,-1,1)\\
1 &= f(0,0,1,-1) + f(1,-1,0,0) + f(1,1,1,1) + f(1,1,-1.-1)\\
1 &= f(1,0,1,0) + f(0,1,0,1) + f(1,1,-1,-1) + f(1,-1,-1,1)
\end{aligned}
$$

There are 11 equations, while each vector occurs an even number of times in them. According to hidden variables postulates, each vector will have a unique pre-assigned value of 0 or 1. However, when summing all the equations, the sum of the left hand side will be odd, but the sum of the right hand side will have to be even, a contradiction. □

3.2 Weak and projective Kochen-Specker sets

Renner and Wolf condensed Kochen-Specker sets to weak Kochen-Specker sets, which are of the smaller size. A *weak Kochen-Specker set* is a subset S of vectors in $\mathbb{C}^n$, such that there for any marking function $S \to \{0,1\}$ there are two orthogonal vectors $u, v \in S$ such that $f(u) = f(v) = 1$. It can easily happen that two vectors are orthogonal, but do not belong to the same basis, if S is a proper subset of $\mathbb{C}^n$.

Every Kochen-Specker set is vacuously a weak Kochen-Specker set, because it has no marking function in the first place. The Renner and Wolf's theorem states that every finite weak Kochen-Specker set can be extended to a Kochen-Specker set.

3.2.1 Theorem. *[25] Let $\mathcal{H} \subseteq \mathbb{C}^d$ and let $S \subseteq \mathcal{H}$ be a finite weak Kochen-Specker set. Then there exists a finite Kochen-Specker set S' such that $S \subseteq S' \subseteq \mathcal{H}$ with*

$$|S' \setminus S| \leq \frac{|S|(|S|-1)}{2}(n-1)$$

Proof. Build S' by extending each pair of orthogonal vectors in S to a basis by adding at most $(n-2)$ vectors to S. Now, S' contains at most

$$\frac{|S|(|S|-1)}{2}(n-1)$$

elements. Now, suppose, there is a marking function on S'. Then, when restricted to S, the function f is still a marking function, so there are two orthogonal vectors $u, v \in S$ such that $f(u) = f(v) = 1$. However, now f evaluates to 1 on two elements in the basis containing u and v in S'. From the contradiction we conclude that S' is a Kochen-Specker set. □

Using projections instead of vectors in the definition of the weak Kochen-Specker sets, Scarpa, Mančinska and Severini generalise the latter to the projective Kochen-Specker sets [18], which Scarpa uses to find a condition for the separation between χ and χ_q in [27].

Definition. A subset $\mathcal{S}$ of $d \times d$ projections over $\mathbb{C}^d$ is a *projective Kochen-Specker set* if for any function $f : \mathcal{S} \to \{0, 1\}$ such that for all subsets $S \subseteq \mathcal{S}$ summing to I_d, that evaluates as follows

$$\sum_{s \in S} f(P_s) = 1,$$

there are two orthogonal projections P and P' in S such that $f(P) = f(P') = 1$.

We could look at the Kochen-Specker sets from the graph theoretic perspective as well by considering orthogonality graphs of the underlying sets. For convenience, using Kernaghan's set of 20 vectors, we would get a 20-vertex orthogonality graph, with the orthogonal bases corresponding to the 4-cliques. If there were a marking function, it would "mark" (or evaluate to one) on one vector from each of these 4-cliques and the chosen vertices would form a coclique. This motivates a definition of a Kochen-Specker graph. A subset of vertices in an orthogonality graph in $\mathbb{R}^d$ is *strictly transverse* if it contains exactly one element from each d-clique. A *Kochen-Specker graph* is an orthogonality graph of the set $S \subseteq \mathbb{R}^3$ such that there exists no strictly transverse subset of the vertices. Just as there are Kochen-Specker set and weak Kochen-Specker sets, we define a *weak Kochen-Specker graph* to be an orthogonality graph of the set $S \subseteq \mathbb{R}^3$ that has no strictly transverse subset that is a coclique. Similarly, projective Kochen-Specker graphs are weak Kochen-Specker graphs with vectors coming from a set of projections, residing in the $\mathbb{C}^d$.

Since in the weak (or projective) Kochen-Specker sets any marking function evaluates to one on two orthogonal items, in such a set the collection of vectors where a marking function evaluates to one will never be a coclique, which motivated our definition.

As expected, if there is a weak Kochen-Specker graph, it is an induced subgraph of a Kochen-Specker graph by the Theorem 3.2.1. Moreover, the Renner and Wolf's construction of completing every pair of orthogonal vertices to a clique, extends a weak Kochen-Specker graph to a Kochen-Specker graph, which is a not disjoint union of d-cliques. If the original graph was finite, the extension will be clearly finite as well. Moreover, we will see this will imply the separation between α and α_q. One instance of this phenomenon is the separation found Teresa Piovesan's Ph.D. thesis [23], which we will see later in 5.4.

Chapter 4

Where classical and quantum chromatic numbers differ

4.1 Introduction

The topic of the quantum chromatic number is relatively well-studied. We are interested in the definitions and graphs with different $\chi(G)$ and $\chi_q(G)$. We will start with the proof of the theorem by Giannicola Scarpa [27, Theorem 3.3.10] that characterises graphs with $\chi < \chi_q$, in terms of projective Kochen-Specker sets representation. In addition, in this chapter we provide new results that generalise Mančinska and Roberson's construction from the "Oddities of quantum colourings" paper [20].

4.2 Relation to the Kochen-Specker sets

The following example due to Giannicola Scarpa is of the fundamental theoretical importance. It relates Kochen-Specker theorem with the separation between the classical and quantum chromatic numbers.

However, it is not easy to check if a set is a Projective Kochen-Specker set: in principle we would have to first identify all the subsets summing to identity, and this is at least as hard as finding all the maximum cliques in the orthogonality graph of the underlying projections, which takes exponential time. Verifying the existence of the marking function will only add complexity.

4.2.1 Theorem. *For all graphs G, we have that $c = \chi_q(G) < \chi(G)$ if and only if the entries $\{P^{(v,i)}\}_{v \in V(G), i \in [c]}$ of the $|V(G)| \times c$ quantum coclique matrix P is a projective KS set.*

Proof. For the forward direction, suppose G is such that $c = \chi_q(G) < \chi(G)$. We will show by contrapositive, that every assignment of quantum colouring projections is a projective Kochen-Specker set. Aiming for a contradiction, we will prove that if $c = \chi_q(G)$ and the union of quantum coclique projections is not a projective Kochen-Specker set, then we can classically c-colour the graph.

Suppose

$$S = \{P^{(v,i)} : v \in V(G), i \in [c]\}$$

is not a projective Kochen-Specker set. Thus, we can find a a marking function $f : S \to \{0, 1\}$ such that for any two orthogonal projections $P, P' \in S$, we either have $f(P) = 0$ or $f(P') = 0$. We claim that

$$\text{colour}(v) = i \text{ if } f(P^{(v,i)}) = 1$$

is a valid classical c-colouring. First, for any two adjacent vertices u and v we have that $P^{(v,i)}P^{(u,i)} = 0$. Since S is a projective Kochen-Specker set, only one of them will be picked, so this is a proper colouring. Each vertex will get a colour, because f, as a marking function, has to evaluate to 1 on all sets of projections summing to I. Thus, $\chi(X) \leq c = \chi_q(G) \leq \chi(G)$, so $\chi(G) = c$, a contradiction.

For the other direction, suppose $\chi_q(G) = c$, and suppose that the union of projections for all quantum colourings form a projective Kochen-Specker set. Towards contradiction, suppose it is possible to colour a graph in c colours. To each v in $V(G)$ with colour β, assign projections $\{P^{(v,i)} = |i + \beta\rangle\langle i + \beta|\}$, where the addition is modulo c. This is a quantum c-colouring, and each vertex gets the same projective measurement, with vertices of different colours having the matrices of this measurement in different orders. Thus, if we define a function

$$f : S \to \{0, 1\}$$
by
$$f(P^{(v,i)}) = \begin{cases} 1 \text{ if } P^{(v,i)} = |1\rangle\langle 1| \\ 0 \text{ otherwise} \end{cases}$$

we can see that f is a marking function that only chooses at most one of any two orthogonal projections. This contradicts the assumption of the union of projections being a projective Kochen-Specker set. □

4.3 Mančinska and Roberson's example

In 2016 Roberson and Mančinska discovered a graph on 14 vertices, for which the quantum chromatic number is less than the classical chromatic number. They conjectured that $\chi(X) = \chi_q(X)$ for any graph X with fewer than 14 vertices. They call the 14-vertex graph G_{14}, which is a cone over G_{13}, a graph defined below.

To define G_{13}, Mančinska and Roberson consider the orthogonality graph of the columns of the matrix below:

$$\begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 1 & 1 & 0 & 0 & 1 & 1 & -1 \\ 0 & 1 & 0 & 1 & -1 & 0 & 0 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & -1 & 1 & -1 & 1 & -1 & 1 \end{bmatrix}.$$

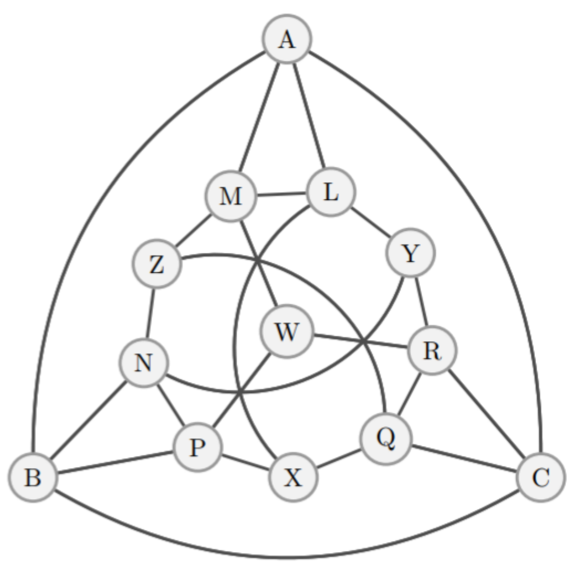

Figure 4.1: G_{13}

Interestingly, Mančinska and Roberson proved that $\chi_q(G_{13}) = \chi_q(G_{14})$. Since we were given a 3-dimensional representation of G_{13}, we can obtain a 4-dimensional representation of G_{14} by appending 0's to the vectors in orthogonal representation of the G_{13}-subgraph and labelling the 14^{th} vertex, called Ω, by $(0,0,0,1)^T$ vector. Using Theorem 2.2.3 Mančinska and Roberson concluded that $\chi_q(G_{14}) \leq 4$. The big portion of the paper is a thorough calculation to show that, in fact,

$$\chi_q(G_{14}) = 4.$$

At the same time, they demonstrated that $\chi(G_{13}) = 4$, implying that

$$\chi(G_{14}) = 5,$$

which gave the desired separation.

In the next section we will attach a more familiar name to G_{13} and generalise this beautiful example.

4.4 Generalisations of Mančinska and Roberson's example

Christopher Godsil observed that the graph G_{13} from [20] is a subgraph of the Erdős-Rényi graph over $GF(3)$, which served as an impetus for generalisation. These graphs have been originally known for having the maximum possible number of edges while not having any 4-cycles, but for us they will serve a new purpose.

For a prime p, the vertices of $ER(p)$ are the one-dimensional subspaces of the vector space $\mathbb{F}_p^3$. We can attach any vector in the subspace to the corresponding vertex. Two such vertices are adjacent if the corresponding vectors are orthogonal over $\mathbb{F}_p^3$. We will explore the version of these graphs with orthogonality relation taken over the reals.

Using the idea of Mančinska and Roberson, there are many ways to build new graphs with the separation of χ and χ_q. One way is to get one instance of orthogonal representation $ER(3)$, which is isomorphic to G_{13}, and then add some 3-dimensional vectors to it. The resulting orthogonality graph will have chromatic number at least 4, because of G_{13} contained in it. At the same time, the cone over it will have a 4-dimensional orthogonal representation, and, thus, quantum chromatic number at most 4, yielding the desired separation. However, not all such constructions will yield even connected examples, as we might choose additional vectors not orthogonal to anything in $ER(3)$, etc.

Here we will demonstrate the promised generalisation, yielding the infinite family of "nice" graphs with the separation between the quantum and classical chromatic numbers.

4.4.1 The chromatic and the quantum chromatic numbers separation in ER(p)

First, construct an orthogonal representation of $ER(p)$ using the 3-dimensional vectors over $\mathbb{Z}_p$ of the form

$$\mathrm{V}(ER(p)) := \{ \left[0, 0, 1\right], \left[0, 1, a\right], \left[1, a, b\right] \}_{a,b \in \{0,\dots,p-1\}} \setminus \{[0, 0, 0]\}.$$

4.4.1 Lemma. *The vectors in $V(ER(p))$ represent all one dimensional subspaces over $\mathbb{F}_p^3$.*

Proof. To see this, first suppose there is a vector $\left[k, c, d\right] \in K, k > 1$ spanning a one-dimensional subspace K. Since $\mathbb{F}$ is a field and $k \neq 0$, there exists $\frac{1}{k} \in \mathbb{F}$. Hence, the vector

$$\left[1, \tfrac{c}{k}, \tfrac{d}{k}\right] \in K,$$

can be viewed as a basis vector for K.

Secondly, suppose, there is a vector $\left[0, m, a\right]$, with $m > 1$ spanning a one-dimensional subspace M. Again, the vector $\left[1, 1, \frac{a}{m}\right]$ is in its span.

Finally, it is clear that any vector of the form $\left[0, 0, a\right]$ is in the span of $\left[0, 0, 1\right]$. □

Now, replace integers $x \in \mathbb{Z}_p$ such that $x > \frac{p-1}{2}$ with $p - x$. In this way, the only entries in the vectors in $\mathrm{V}(ER(p, 3))$ will be

$$0, \pm 1, \dots, \pm \frac{p-1}{2}.$$

Now, construct an orthogonality graph over $\mathbb{R}$ using this form of $\mathrm{V}(ER(p))$, and call this graph $ER'(p)$. Note that $ER'(3)$ is just G_{13}.

4.4.2 Lemma. *$ER'(p)$ with the above representation over $\mathbb{R}$ is connected.*

Proof. We will show that between any pair of vertices there exists a path. To begin, assume $b \neq 0, d \neq 0$.

First, consider a pair of vertices of $ER'(p)$: vertex $\left[0,a,b\right]$ and $\left[0,c,d\right]$ such that $a, b \in \{0, \pm 1, ..., \pm \frac{p-1}{2}\}$. Then there is a path consisting of vertices:

$$\left[0,a,b\right], \left[1,0,0\right], \left[0,c,d\right].$$

Now look at a different pair of vertices of $ER'(p)$: vertex v, labelled by $\left[0,a,b\right]$ and u, labelled by $\left[1,c,d\right]$ such that $a, b \in \{0, \pm 1, ..., \pm \frac{p-1}{2}\}$. Then there is a path consisting of vertices:

$$\left[0,a,b\right], \left[1,0,0\right], \left[0,1,-\tfrac{c}{d}\right], \left[0,c,d\right].$$

Finally, between the vertices $[1,a,b]$ and $[1,c,d]$ there is a path

$$[1,a,b], [0,1,-\frac{a}{b}], [1,0,0], [0,1,-\frac{c}{d}], [1,c,d].$$

Now, in case $b = 0, d = 0$ there will be a path

$$\left[1,a,0\right], \left[0,0,1\right], \left[1,c,0\right].$$

If only one of b, d is 0, without loss of generality assume $b = 0, d \neq 0$, then there will be a path

$$\left[1,a,0\right], \left[0,0,1\right], \left[1,0,0\right], \left[0,1,-\tfrac{c}{d}\right], \left[0,c,d\right].$$

These represent all the most general pairs of vertices, so we conclude that the graph is connected. □

4.4.3 Lemma. $\chi(ER'(p)) \geq 4$.

Proof. Since $ER'(3)$ is the orthogonality graph of the subset of $V(ER'(p))$,

$$\chi(ER'(p)) \geq \chi(ER'(3)) = \chi(G_{13}) \geq 4.$$

□

The above lemma shows that the cone over $ER'(p)$ will have the separation between the χ and χ_q. This is not the only way to construct such graphs. We need to be careful about the construction. For example, as in G_{13} over $\mathbb{Z}_3$, we had vertices $(1,1,0)$ and $(1,-1,0)$ orthogonal over $\mathbb{Z}_3$ and over $\mathbb{R}$. However, if we chose the embedding where the vectors will be not as above, but, say, $(1, 1, 0)$ and $(1, 2, 0)$ instead, the orthogonality over $\mathbb{R}$ would have been lost. In general, we can chose a very specific set of entries for the vectors, $0, \pm 1, ..., \pm \frac{p-1}{2}$, which guarantees that the orthogonality graph over $\mathbb{R}$ will be connected. However, any choice of integers, as long as it includes $0, \pm 1$ will work for the proof of the above lemma, but may result in the disconnected graph. Only the connected component containing G_{13} may be considered.

Using similar ideas, we could construct $ER'(p, 4)$, with vertices being one-dimensional subspaces of $\mathbb{R}^4$. Technically, it will have no right to be called Erdős-Rényi any more, but will contain G_{14} now, the cone over G_{13}, and will also yield the separation.

Chapter 5

Where classical and quantum coclique numbers differ

5.1 Introduction

There are few currently known examples of graphs where classical coclique number is strictly less than the quantum one. One can be found in Teresa Piovesan's Ph.D thesis [23, Page 34]. Another construction by Giannicola Scarpa [27, Section 3.4.2] allows to construct a graph with $\alpha < \alpha_q$, given a graph where $\chi > \chi_q$. There is also a construction by Mančinska and Roberson [21] based on the differences between quantum and classical homomorphisms.

In this chapter we will prove a characterisation of separation for quantum cocliques using projective Kochen-Specker sets. Teresa Piovesan's example is also based on Kochen-Specker sets. Therefore, it is logical to start with a section submerging a reader into the background on Kochen-Specker theorem.

5.2 Relation to the Kochen-Specker sets

Very interestingly, we were able to discover that there is a similar characterisation of the independence numbers' separation, as in the case with chromatic numbers. However, as the statement resembles an analogous result about the chromatic number, the same complexity issues arise. It is at least exponentially difficult to check if the given set of projections is a projective Kochen-Specker set, if one had to identify all sets of projections summing to identity first. The reason is that identifying all sets of projections summing to identity is equivalent to finding all maximum cliques in the orthogonality graph of the all $\alpha_q|V(G)|$ coclique assignment projections of the graph G.

5.2.1 Theorem. *For all graphs G, we have that $k = \alpha_q(G) > \alpha(G)$ if and only if the entries $\{P^{(v,i)}\}_{v \in V(G), i \in [k]}$ of the $|V(G)| \times k$ quantum coclique matrix P form a projective KS set.*

Proof. For the forward direction, suppose that $k = \alpha_q(G) > \alpha(G)$. With a contrapositive technique, we will prove that if there is a quantum coclique assignment that is not a projective Kochen-Specker set, we will be able to find a classical coclique in G of size k.

If $S = \{P^{(v,i)} : v \in V(G), i \in [k]\}$ is a quantum coclique assignment in dimension d that is not a projective Kochen-Specker set, then there is a marking function

$$f : S \to \{0, 1\}$$

such that for any pair of two orthogonal projections P, P' at most one gets marked, i.e. either $f(P) = 0$ or $f(P') = 0$. Now, let

$$S_i := \{P^{(v,i)} : v \in V(G), 1 \leq i \leq k\}.$$

Then

$$\sum S_1 = \sum_{v \in V(G)} P^{(v,1)} = I_d \quad (1)$$

$$\vdots$$

$$\sum S_k = \sum_{v \in V(G)} P^{(v,k)} = I_d \quad (k).$$

From the definition of quantum coclique within the same vertex row of the corresponding $|V(G)| \times \alpha_q$ matrix all projections will be orthogonal.

Now, use a marking function f to find a classical k-coclique K, according to the rule:

$$\text{if } f(P^{(v,i}) = 1 \text{ for some } i \in [k], \text{ include } v \text{ into } K \qquad (*)$$

We will see that this chooses a classical coclique of size k. First, recall from the definition of quantum coclique that if u and v are adjacent, then $P^{(v,i)}P^{(u,j)} = 0$ for any $i, j \in [k]$. Therefore, since S is not a projective

Kochen-Specker set and f is a marking function, f can only choose one projection per vertex, and at most one projection will be chosen from any pair of adjacent vertices. Thus, the set of vertices chosen by the $(*)$ rule, say $K' = \{v_1, ..., v_m\}$ is a coclique. In order for f to be a marking function, it has to choose at least one projection from each S_t since $\sum S_t = I_d$, so it will choose a classical coclique of size k. Now $k \leq \alpha(G) \leq \alpha_q(G) = k$, so $\alpha(G) = k$, a contradiction.

For the other direction, suppose that $\alpha_q(G) = k$, and every quantum coclique assignment

$$S_i := \{P^{(v,i)} : v \in V(G), i \in [k]\}$$

is a projective Kochen-Specker set. Towards contradiction, we assume that $\alpha(G) = k = \alpha_q(G)$. Now let $K = \{v_1, ..., v_k\}$ be a classical coclique of size k in G. To each $v_t \in K$ assign a tuple of projections $\{P^{(v_t,i)}\}_{i\in[k]}$ such that only $P^{(v_t,t)}\}$ is nonzero. Let $\{P^{(v_t,t)}\} = I_d$. For vertices in G that are not in K, assign k-tuples of 0 projections. This is a valid k-quantum coclique assignment. Moreover, consider the function $f : S \to \{0, 1\}$

$$f(P^{(v,i)}) = \begin{cases} 1 & \text{if } P^{(v,i)} = I_d \\ 0 & \text{otherwise} \end{cases}$$

For each S_i it evaluates to 1, and whenever two projections are orthogonal, f picks at most one of them. Thus, f is a marking function, contradicting the fact that S is a projective Kochen-Specker set. □

As we have discussed in the first chapter, the notions of chromatic number and independence number are classically related. We have been looking for something connecting their quantum counterparts. The reliance on projective Kochen-Specker sets in order to exhibit the separation provides one new link between quantum chromatic and independence numbers.

We will open the following section with Scarpa's theorem which provides another relation between the quantum chromatic and independence numbers.

5.3 Giannicola Scarpa's construction

In search for quantum and classical independence numbers separation and having many graphs with chromatic numbers' separation on hand, it is natural to inquire if the found examples of $\chi_q < \chi$ can give rise to graphs with

$\alpha < \alpha_q$. It turns out, there is a connection, involving Cartesian products of graphs. Scarpa found a relevant graph and proved the separation by establishing an upper bound for its classical independence number and a strictly greater lower bound for its quantum one.

Definition (Cartesian product of graphs)**.** Cartesian product of graphs G and H, denoted $G\Box H$, has the vertex set $V(G) \times V(H)$, and vertices (x_1, h_1) and (x_2, h_2) are adjacent if either $x_1 = x_2$ and $h_1 \sim h_2$, or $h_1 = h_2$ and $x_1 \sim x_2$.

5.3.1 Lemma ([14])**.** *Let G be a graph on n vertices with $\chi(G) > k$. Then we have $\alpha(G\Box K_k) < n$.*

Proof. Observe that $G\Box K_k$ can be partitioned into n disjoint cliques K_k. Towards contradiction, suppose that $\alpha(G\Box K_k) \geq n$. We can only pick at most one vertex from each of the n cliques, so suppose $\alpha(G\Box K_k) = n$ and $W \subsetneq V$ is an independent set of size n.

Now, properly colour $G\Box K_k$ as follows. If a vertex $(v, i), 1 \leq i \leq k$ belongs to W, colour it with a colour i. Now, vertices of same colour (v, i) and (u, i) are adjacent if and only if $u \sim v$ in G and they are in the same clique K_k, and, thus, not both of them in W. Therefore, restricted to only the vertices of G, this is a proper colouring of G with k colours, contradicting that $\chi(G) > k$.

□

Now we will proceed to the construction.

5.3.2 Theorem ([27])**.** *Let G be a graph such that $k = \chi_q(G) < \chi(G)$, then $\alpha_q(G\Box K_k) > \alpha(G\Box K_k)$.*

Proof. Consider a graph G with some quantum colouring with k colours. Suppose, the v^{th} row of the corresponding $|V(G)| \times k$ matrix has projections $\{P^{(v,i)}\}_{i\in[k]}$. Construct G' with vertices $(v, i), v \in V(G), i \in [k]$. Construct its quantum n-colouring such that the row corresponding to (v, i) of the quantum colouring matrix has $n - 1$ zero projections, while only the v^{th} column has the projection $P_i^{(v)}$. Declare (v, i) and (u, j) to be adjacent whenever their nonzero projections are orthogonal. The resulting graph G' will have n cliques of size k. The at most k nonzero projections in such a clique will come from the k-quantum colouring of some vertex of G and thus will sum to identity. Note that the given projections satisfy the definition of quantum coclique, so $\alpha_q(G') \geq n$.

Consider the relationship between (v,i) and (u,i). They are adjacent if and only if $v \sim u$ in G because $P^{(v,i)}P^{(u,i)} = 0$. Similarly, (v,i) and (v,j) are adjacent whenever i and j are different. No other cases of adjacency exist. Therefore, the created graph G' is $G \square K_k$.

If we choose G such that $k = \chi_q(G) < \chi(G)$ and build $G \square K_k$ as above, we are going to obtain a graph with $\alpha(G \square K_k) < n$ by Lemma 5.3.1 and $\alpha_q(G \square K_k) \geq n$. □

5.4 Teresa Piovesan's example

One example when $\alpha < \alpha_q$ comes from Teresa Piovesan's thesis at page 34 [23]. The author used a Kochen-Specker graph G_p from [8] to prove the separation.

We provide the underlying Kochen-Specker set G_p below and explain how the separation is achieved.

1: (1,0,0,0)	2: (0,1,0,0)	3:(0,0,1,0)	4: (0,0,0,1)
5: (0,1,1,0)	6: (1,0,0,-1)	7: (1,0,0,1)	8: (0,1,-1,0)
9: (1,1,1,1)	10: (1,-1,1,-1)	11: (1,-1,-1,1)	12: (1,1,-1,-1)
13: (1,-1,0,0)	14: (1,1,0,0)	15: (0,0,1,1)	16: (0,0,1,-1)
17: (-1,1,1,1)	18: (1,1,1,-1)	19: (1,-1,1,1)	20: (1,1,-1,1)
21: (1,0,1,0)	22: (0,1,0,1)	23: (1,0,-1,0)	24: (0,1,0,-1)

Each row of this table forms an orthonormal basis. Therefore, the sets of vertices

$$V_1 = \{1,2,3,4\}, V_2 = \{5,6,7,8\}, V_3 = \{9,10,11,12\},$$
$$V_4 = \{13,14,15,16\}, V_5 = \{17,18,19,20\} V_6 = \{21,22,23,24\}$$

partition $V(G)$ into six cliques.

We will first establish the upper bound on the classical coclique number. To choose vertices for a coclique in G_p, one has to choose at most one vertex from each of the six cliques. The set of bases that form these cliques was chosen in [8] to be a Kochen-Specker basis set. In other words, it is impossible to choose six elements, one from each of the bases, such that pairwise they are non-orthogonal. In terms of orthogonal representation, it means that there is no coclique of size six in G_p, so $\alpha(G_p) < 6$.

Now, consider the following construction from [23] of the projections for quantum coclique. For a vertex u in a clique V_j we assign

$$P^{(u,i)} = 0 \text{ for } i \in [6] \setminus j$$

and

$$P^{(u,j)} = x_u x_u^T,$$

where x_u is the normalised vector of u. Such projections will satisfy the definition of quantum coclique . Now, each vertex gets assigned six projections, so $\alpha_q \geq 6$.

5.4.1 Lemma. *The maximal cliques of G_p have size four. Moreover, every pair of adjacent vertices in the above orthogonality graph G_p is in some maximal 4-clique.*

Proof. Can be easily checked computationally. □

In particular, this property forces this set of vectors with orthogonality adjacency rule to be a Kochen-Specker set.

Chris Godsil has suggested a description of G_p in terms of Cayley graphs.

Definition. [13, Section 3] The Cayley graph $Cay(G, C)$ is the graph with vertex set consisting of elements of a group G and edge set

$$E(\mathrm{Cay}(G, C)) = \{gh : hg^{-1} \in C\}$$

In the following two theorems we will see the isomorphism. The first theorem establishes it, while the second one will reveal mysterious underlying quaternionic behaviour of the bijection.

5.4.2 Lemma. *Piovesan's graph G_p is isomorphic to a Cayley graph of a symmetric group on 4 letters with the connection set of elements of order 2.*

Proof. One can check that the following assignment is an isomorphism:

1: ()	2: (12)(34)	3:(13)(24)	4: (14)(23)
5: (23)	6: (1243)	7: (1342)	8: (14)
9: (124)	10: (234)	11: (143)	12: (132)
13: (1324)	14: (1423)	15: (34)	16: (12)
17: (142)	18: (134)	19: (123)	20: (243)
21: (1432)	22: (13)	23: (1234)	24: (24).

5.4.3 Theorem. *There is an orthogonal representation of G_p, similar up to a sign to the one given above, such that it is isomorphic to* Cay(S_4, C), *where* $C := \{s \in S_4 : s^2 = ()\}$.

Proof. Chris Godsil has observed that according to the embedding in the Lemma 5.4.2, the cliques $B_2, ..., B_6$ are the cosets of the group formed by the elements of $\{(),(12)(34),(13)(24),(14)(23)\}$ of S_4. It is therefore reasonable to assign standard basis vectors to them as follows:

$$\begin{aligned} () &\to e_1 \\ (12)(34) &\to e_2 \\ (13)(24) &\to e_3 \\ (14)(23) &\to e_4 \end{aligned}$$

This is an arbitrary assumption, but building on it below we will see how it is useful. We will show how to obtain the rule for multiplication of e_i's, and we'll evidence how resembles the Quaternion structure. First, we will show that if $i \neq j$, then $e_i e_j \notin \{e_1, e_i, e_j\}$. From the above assignment we have that

$$e_i e_j \notin \{e_i, e_j\}.$$

To show that for $i \neq j$ we have $e_i e_j \neq e_1$, suppose by contradiction that

$$\begin{aligned} e_i e_j &= e_1 \\ e_i e_j e_j = e_1 e_j &= e_j \\ \pm e_i &= e_j, \end{aligned}$$

which is false. Additionally, we will assume that $e_i^2 = -e_i$ for $i = 2, 3, 4$.

Since every permutation can be written as a product of transpositions, we will represent them in terms of vectors first. We illustrate the general procedure with one example. The other cases will be analogous.

$$\begin{aligned} (14) &= ae_1 + be_2 + ce_3 + de_4, \quad a, b, c, d \in \mathbb{R} \\ (23) &= xe_1 + ye_2 + ze_3 + we_4, \quad x, y, z, w \in \mathbb{R} \end{aligned}$$

Using our assumption that $(14)(23) = e_4$, we construct the system of equations:

$$\begin{cases} (14) = [(14)(23)](23) \\ (23) = (14)[(14)(23)] \end{cases}$$

$$\begin{cases} ae_1 + be_2 + ce_3 + de_4 = e_4(xe_1 + ye_2 + ze_3 + we_4) \\ xe_1 + ye_2 + ze_3 + we_4 = (ae_1 + be_2 + ce_3 + de_4)e_4 \end{cases}$$

Using that $e_4^2 = -1$

$$\begin{cases} ae_1 + be_2 + ce_3 + de_4 = xe_4 + ye_4e_2 + ze_4e_3 - we_1 \\ xe_1 + ye_2 + ze_3 + we_4 = ae_4 + be_2e_4 + ce_3e_4 - de_1 \end{cases}$$

We obtain:

$$\begin{cases} a = -w \\ d = x \\ ce_3 = ye_4e_2 \\ be_2 = ze_4e_3 \\ x = -d \\ w = a \\ ye_2 = ce_3e_4 \\ ze_3 = be_2e_4 \end{cases}$$

Clearly, $a = d = w = x = 0$.

$$\begin{cases} ce_3 = ye_4e_2 \\ be_2 = ze_4e_3 \\ ye_2 = ce_3e_4 \\ ze_3 = be_2e_4 \end{cases}$$

$$\begin{cases} ye_2e_4 = c_3e_4e_4 = -ce_3 = -ye_4e_2 \\ ze_3e_4 = be_2e_4e_4 = -be_2 = -ze_4e_3 \\ ce_3e_2 = ye_4e_2e_2 = -ye_4 = -ce_3e_2 \end{cases}$$

We established that if $i \neq j$, then $e_ie_j \notin e_1, e_i, e_j$, we conclude that

$$\begin{aligned} e_4e_3 &= e_2 = -e_3e_4 \\ e_2e_4 &= e_3 = -e_4e_2 \\ e_3e_2 &= e_4 = -e_2e_3 \\ e_ie_1 &= e_1e_i \text{ for } i = 2, 3, 4 \\ e_i^2 &= -e_1 \end{aligned}$$

The signs are arbitrary, and depending on which choice of signs one has, the embedding will be different. Moreover, for convenience we choose integers mod 3 as coefficients, and we have that

$$
\begin{aligned}
(14) &= e_2 - e_3 \\
(23) &= e_2 + e_3
\end{aligned}
$$

Similarly,

$$
\begin{aligned}
(13) &= e_2 + e_4 \\
(24) &= e_2 - e_4 \\
(12) &= e_3 - e_4 \\
(34) &= e_3 + e_4
\end{aligned}
$$

To construct representations for all other permutations, write them canonically as a product of transpositions, and use the above-mentioned rules for the multiplication of e_i's. □

5.4.1 New separation between α and α_q

Using this idea, we construct a graph G_{120} on 120 vertices labelled by the elements of S_5 with the separation between $29 = \alpha(G_{120})$ and $\alpha_q(G_{120}) \geq 30$. To start, assign every vertex of $S_4 \subseteq S_5$ the same 4-dimensional vector as above.

Using the procedure outlined above, when searching for the homomorphism between G_p and the Cayley graph, and writing all permutations involving 5 as a product of transpositions, we can find 4-dimensional vectors corresponding to the vectors in S_5 but not S_4. However, first we need to decide how the transposition in S_5 but not S_4 are represented. Here is the example of this procedure with $(1,5)$. Transpositions $(2,5)$, $(3,5)$ and $(4,5)$ will be analogous.

We want a vector corresponding $(1,5)$ to be adjacent to the vectors corresponding to

$$
\begin{aligned}
(2,3) &= (1,5)\dot{(}1,5)(2,3) \\
(2,4) &= (1,5)\dot{(}1,5)(2,4)
\end{aligned}
$$

$$(3,4) = (1,5)\dot{(}1,5)(3,4)$$

in the orthogonality graph. From the above calculations we had that

$$(2,3) \to e_2 + e_3$$
$$(2,4) \to e_2 - e_4$$
$$(3,4) \to e_3 + e_4$$

Now, let $(1,5)$ correspond to $ae_1 + be_2 + ce_3 + de_4$. Then

$$(ae_1 + be_2 + ce_3 + de_4) \cdot (e_2 + e_3) = b + c = 0$$
$$(ae_1 + be_2 + ce_3 + de_4) \cdot (e_2 - e_4) = b - d = 0$$
$$(ae_1 + be_2 + ce_3 + de_4) \cdot (e_3 + e_4) = c + d = 0$$

Therefore, $(1,5)$ corresponds to a vector $(*, b, -b, b)$. Let us choose $(0,1,-1,1)$. In general, let us use vectors in this representation of S_5.

(15) to correspond to a vector $(0,1,-1,1)$,
(25) to correspond to a vector $(0,1,1,-1)$,
(35) to correspond to a vector $(0,1,1,1)$,
(45) to correspond to a vector $(0,-1,1,1)$

Now we will use the vectors assigned to all the elements of S_5 to construct orthogonality graph G_{120}. Turns out, G_{120} can be partitioned into 30 cliques of size 4, resulting into the lower bound $\alpha_q(G) \geq 30$. Computationally, one will be able to check that $\alpha(G) = 29$. Interestingly, the resulting graph is not Cayley and the Piovesan's graph $G_p = \mathrm{Cay}(S_4, \text{involutions})$ is not its subgraph.

5.5 Mančinska and Roberson's construction - homomorphic product

Now we will need to recall the definition of quantum homomorphisms. Since the classical independence number can be expressed in terms of homomorphisms, and α_q can be defined with quantum homomorphisms, there is a hope for the separation between α and α_q if the quantum homomorphism exists between K_t and X, but the classical one does not. In [21], Mančinska and Roberson show that any graphs for which $X \to Y$ but $X \overset{q}{\nrightarrow} Y$ can be used to construct graphs for which $\alpha_q > \alpha$. First we need some lemmas and definitions.

We begin with a folklore definition of the homomorphic product, relations of which mimic relations between (x, y)-vertex-labelled projections in the definition of the quantum homomorphism between the graphs X and Y.

Definition (Homomorphic product)**.** For graphs X and Y, the *homomorphic product* $X \ltimes Y$ is the graph with vertex set $V(X) \times V(Y)$ with distinct vertices (x, y) and (x', y') adjacent if either $x = x'$, or $x \sim x'$ and $y \nsim y'$.

The next lemma demonstrates why homomorphic product can be useful, and, probably, why it is called so.

5.5.1 Lemma. *For graphs X and Y, we have that $X \to Y$ if and only if $\alpha(X \ltimes Y) = |V(X)|$*

Proof. Follows easily from the definition of the homomorphic product □

.

The quantum analogue holds true as well, for which we do not include the proof. It can be found in the Mančinska and Roberson's paper in [21].

5.5.2 Lemma. *For graphs X and Y, we have that $X \xrightarrow{q} Y$ if and only if $\alpha_q(X \ltimes Y) = |V(X)|$*

From the above two lemmas Lemma 5.5.1 and Lemma 5.5.2, we have the following.

5.5.3 Corollary. *If $X \nrightarrow Y$ and $X \xrightarrow{q} Y$, then $\alpha(X \ltimes Y) < \alpha_q(X \ltimes Y)$*

Proof. If $X \nrightarrow Y$ then $\alpha(X \ltimes Y) < |V(X)|$. However, if $X \xrightarrow{q} Y$, then $\alpha_q(X \ltimes Y) = |V(X)|$. □

In their paper [20], Mančinska and Roberson have proved that the graph G_{13} has $4 = \chi(G) = \chi_q(G)$. This graph is an orthogonality graph of a Kochen-Specker set [30]. What was interesting is that in G_{14}, obtained by adding an apex vertex to G_{13}, quantum chromatic number remained unchanged, $\chi_q(G_{14}) = 4$, but $\chi_q(G) = 5$ certainly went up. Thus G_{14} exhibited the separation between χ and χ_q.

So far all the known examples exhibiting separation between α and α_q also exhibited separation between χ and χ_q and were orthogonality graphs of a Kochen-Specker set. They had chromatic number 5 and a 4-dimensional orthogonal representation, where the latter implied that $\chi_q \leq 4$ (Proposition 12 in [7]. It is, therefore, natural to check whether G_{14} exhibits separation between α and α_q. However, according to the theorem 2.4.2, since $\alpha_q(G_{13}) = \alpha_q(G_{14})$, so we only need to check $\alpha_q(G_{13})$. We will show that unlike the most examples coming from Kochen-Specker sets, this one does not have both separations. To prove it, we will need the definition of Lovász ϑ.

Definition ([17])**.** Let $G = (V, E)$ be a graph, and let $\mathcal{M}(G)$ denote the set of $V \times V$ symmetric matrices A such that $A_{ii} = 1$ for all $i \in V$ and $A_{ij} = 1$ for $i \neq j$ and $ij \notin E$. Let $\lambda_{\max}(A)$ denote the largest eigenvalue of a symmetric matrix A. We have that for any graph G,

$$\vartheta(G) = \min_{A \in \mathcal{M}(G)} \lambda_{\max}(A).$$

5.5.4 Theorem. $\alpha(G_{13}) = \alpha_q(G_{13}) = 5$.

Proof. Lovász ϑ is an upper bound for α_q [5]:

$$5 = \alpha(G_{13}) \leq \alpha_q(G_{13}) \leq \vartheta(G_{13}).$$

The last inequality comes from [17]. Now, consider the matrix A, where

$$\begin{aligned} A_{ii} &= 1 \text{ for all } i \in V(G) \\ A_{ij} &= 1 \text{ for all } uv \notin E(G) \\ A_{uv} &= -1.24 \text{ for all } uv \in E(G) \end{aligned}$$

This matrix satisfies the definition for $\nu(G)$ and its largest eigenvalue is < 5.7. Thus, $\alpha_q(G) \leq 5$, and $\alpha_q(G) = \alpha(G) = 5$. $\square$

Chapter 6

Inertia and Lovász ϑ upper bounds on α_q

In this chapter we will look at the proofs of some tremendously helpful known upper bounds for α_q, which are also bounds on α. There has been a proof of the inertia bound in [29] and an indirect proof of the Lovász ϑ in a number of papers. We will give a direct proof here, which relies on the idea from [5].

Since $\alpha \leq \alpha_q$, the cases when at least one of these bounds is within less than one away from α have no quantum versus classical independence number separation. Checking if this is the case is usually the first procedure to follow when trying to find a separation, taking advantage of the fact that both bounds can be determined in polynomial time.

6.1 Inertial upper bound for the classical independence number

Wocjan and Elphick [29] establish an inertia bound on the quantum independence number based on Godsil's [12] proof of the classical analogue. We are going to prove this below, but first we will need to introduce a new matrix associated with a graph. *Hermitian adjacency matrices* were originally defined for directed graphs to encode the number of edges between vertices.

The weighted Hermitian adjacency matrix H of a digraph D is defined by

$$H_{u,v} = \begin{cases} \mathbf{i}w \text{ if there is an arc from } u \text{ to } v \\ -\mathbf{i}w \text{ if there is an arc from } v \text{ to } u \\ w \text{ if there are arcs from } u \text{ to } v \text{ and from } v \text{ to } u \\ 0 \text{ otherwise.} \end{cases}$$

6.1.1 Theorem (Classical inertia bound)**.** *Suppose, W is a Hermitian weighted adjacency matrix of G and $n^0(W), n^+(W), n^-(W)$ are the numbers of its zero, positive and negative eigenvalues respectively. Then the following holds:*

$$\alpha(G) \leq n^0(W) + \min\{n^+(W), n^-(W)\}.$$

□

The authors use Godsil's proof from [12], but first they prove a useful lemma, on which the proof relies.

6.1.2 Lemma. *Let $M \in \mathbb{C}^{m\times m}$ be an arbitrary Hermitian matrix. A subspace U of $\mathbb{C}^m$ is called totally isotropic with respect to the Hermitian form defined by M if*

$$u^* M u = 0$$

for all vectors $u \in U$. The dimension of all maximally totally isotropic subspaces is equal to

$$n^0(M) + \min\{n^+(M), n^-(M)\}$$

Proof. The matrix M is Hermitian, so by spectral decomposition, we can find invertible matrix S and a diagonal matrix D, such that

$$D = SAS^T.$$

By Sylvester's law of inertia, the number of negative elements in the diagonal of D is always the same, for all such S, and the same holds for the number of positive elements. With this rule, we can simplify the statement and let M be diagonal. By scaling if necessary, we may further assume that it has only eigenvalues $+1, 0, -1$.

We proceed by finding a totally isotropic subspace of the specified dimension

$$n^0(M) + \min\{n^+(M), n^-(M)\}.$$

Let x_a^+, x_b^0 and x_c^- be the eigenvectors of M with corresponding eigenvalues $1, 0$ and -1, and assume $a = 1, ..., n^+, \quad b = 1, ..., n^0$ and $c = 1, ..., n^-$. Assuming without loss of generality that $n^+ \geq n^-$, the subspace U spanned by

$$\begin{aligned} x_b^0, &\quad b \in [n^0], \\ x_c^+ + x_c^-, &\quad c \in [n^-] \end{aligned}$$

is indeed such that $e_u^T M e_u = 0$ for all $u \in U$, so it is totally isotropic of dimension $n^0 + n^-$, which by assumption is $n^0 + \min\{n^-, n^+\}$.

It is left to show that no other totally isotropic subspace can be of a larger dimension. Let U be any totally isotropic subspace and V be a subspace spanned by $x_a^+, a \in [n^+]$. It follows that since both U and V are subspaces of the eigenspace of M,

$$\begin{aligned} n^+ + n^- + n^0 &= m \\ &\geq \dim(U + V) \\ &= \dim(U) + \dim(V) - \dim(U \cap V) \\ &= \dim(U) + n^+. \end{aligned}$$

The last equality follows from the fact that $\dim(U \cap V) = 0$. Indeed, since V is spanned by the eigenvectors of M with positive eigenvalues, if $x \in V$, then $x * Mx \neq 0$. Moving n^+ to the left, we see that $\dim(U) \leq n^0 + n^-$. □

Now we are ready to prove the classical inertia bound Theorem 6.1.1.

Proof. First, G be a graph with a weighted adjacency matrix W. If two vertices u, v are non adjacent in G and their corresponding basis vectors are e_u and e_v, then

$$e_u W e_v = W_{u,v} = 0.$$

In other words, by associating standard basis vectors in $|V(G)|$ dimensions, we identify each coclique $S \subseteq V(G)$ with a totally isotropic subspace of dimension $|S|$. The inertia bound thus follows from the Lemma 6.1.2. □

6.2 Inertial upper bound for the quantum independence number

In this section we will present inertial upper bound of Wocjan and Elphick [29] on quantum independence number. The end goal is to prove the following.

6.2.1 Theorem. *For any graph G with quantum independence number $\alpha_q(G)$ and Hermitian weighted adjacency matrix W:*

$$\alpha_q(G) \leq n^0 + \min\{n^+(W), n^-(W)\}.$$

□

This lemma is an elementary linear algebraic result linking orthogonality of projections, needed for α_q, and the spectral decomposition, related to the inertia bound.

6.2.2 Lemma. *Let $P, Q \in \mathbb{C}^{d\times d}$ be two arbitrary orthogonal projectors of rank r and s, respectively. Let*

$$P = \sum_{k\in[r]} x_k x_k^T \text{ and } Q = \sum_{t\in[s]} y_t y_t^T$$

denote their spectral decompositions. Then the following are equivalent:

(a) $\langle P, Q\rangle_{\mathrm{tr}} = 0$

(b) $x_k^T y_t = 0$ *for all* $k \in [r]$ *and* $l \in [s]$

Proof. The backwards direction is trivial. The forward direction follows from the fact that each $x_k x_k^T$ and $y_t y_y^T$ is positive semidefinite. Since the product of two symmetric positive semidefinite matrices is positive semidefinite, $0 = \langle P, Q\rangle_{\mathrm{tr}}$ is a sum of positive semidefinite matrices, which implies that each summand is a 0-matrix. □

Now, recall the indexing of the projections in the definition of quantum coclique number. For each $P^{(u,i)}$, define spectral decomposition vectors $x_k^{(u,i)}$, so that

$$P^{(u,i)} = \sum_{k\in[r^{(u,i)}]} x_k^{(u,i)} (x_k^{(u,i)})^T.$$

The following counting result will help to establish the upper bound on the dimension of the maximum isotropic subspace.

For $u \in V, i \in [t], k \in [r^{(u,i)}]$, define the composite vectors

$$\psi_k^{(u,i)} = e_u \otimes x^{(u,i)} \in \mathbb{C}^{n\times n} \otimes \mathbb{C}^{n\times n},$$

6.2.3 Lemma. *The cardinality of the index set*

$$\{(u,i,k) : u \in V(G), i \in [t], k \in [r^{(u,i)}]\} \qquad (1)$$

is td.

Moreover, for all $u, v \in V, k, l \in [t], k \in [r^{(v,j)}]$, *we have :*

$$\begin{aligned} \langle \psi_k^{(u,i)}, \psi_l^{(v,j)} \rangle &= \delta_{u,v}\delta_{i,j}\delta_{k,l} \\ (\psi_k^{(u,i)})^T (A \otimes I_d) \psi_l^{(v,j)} &= 0. \end{aligned}$$

Proof. From the definition of quantum coclique we are guaranteed that

$$\sum_{u \in V(G)} P^{(u,i)} = I_d.$$

In addition, the projections $P^{(u,i)}$ for $i \in [t]$ are pairwise orthogonal, which implies that their ranks are additive:

$$\sum_{u \in V(G)} r^{(u,i)} = d, \text{ for each } i \in [t].$$

For a fixed $u \in V(G)$ the only variable parameters in $\psi_k^{(u,i)}$ are $i \in [t]$ and $k \in [r^{(u,i)}]$, which proves (1).

Now,

$$\begin{aligned} \langle \psi_k^{(u,i)}, \psi_l^{(v,j)} \rangle &= e_u^T e_v \otimes (x_k^{(u,i)})^T (x_l^{(v,j)}) \\ &= \delta_{u,v} (x_k^{(u,i)})^T (x_l^{(v,j)}) \\ &= \delta_{u,v} \langle x_k^{(u,i)}, x_l^{(v,j)} \rangle \end{aligned}$$

It remains to investigate

$$\langle x_k^{(u,i)}, x_l^{(u,j)} \rangle = \mathrm{tr}(x_k^{(u,i)})^T (x_l^{(u,j)}) \qquad (*)$$

Again, from the definition of quantum coclique, $P^{(u,i)}P^{(v,j)} = 0$ if $i \neq j$, which by Lemma 6.2.2 means $(*)$ is 0. Furthermore, if $i = j$, but $k \neq l$ we observe that $x_k^{(u,i)}$ and $x_l^{(u,j)}$ form orthogonal spectral idempotents of $P^{(u,j)}$, which again makes $(*)$ is 0 by Lemma 6.2.2 . It follows that

$$\langle \psi_k^{(u,i)}, \psi_l^{(u,j)} \rangle = \delta_{i,j}\delta_{k,l}.$$

To prove the rest, note that

$$(\psi_k^{(u,i)})^T(A \otimes I_d)\psi_l^{(v,j)} = (e_u^T \otimes (x_k^{(u,i)})^T)(A \otimes I_d)(e_v \otimes (x_k^{(v,i)}))$$
$$= e_u^T A e_v^T \otimes (x_k^{(u,i)})^T(x_k^{(v,i)})) = e_u^T A e_v^T \langle x_k^{(u,i)}, x_k^{(v,i)} \rangle$$

If $uv \notin E(G)$, the first part of the tensor product in the last equality will be 0 by the quantum coclique definition and Lemma 6.2.2 and we are done.

Now suppose, $uv \in E(G)$, and suppose $i \neq j$. It follows that

$$\langle x_k^{(u,i)}, x_k^{(v,j)} \rangle = \langle P^{(u,i)}, P^{(v,j)} \rangle = 0.$$

Finally, suppose that $uv \in E(G)$, and suppose $i = j$, then

$$\langle x_k^{(u,i)}, x_k^{(v,i)} \rangle = \langle P^{(u,i)}, P^{(v,i)} \rangle = 0.$$

Last two equalities again follow from the definition of quantum coclique and Lemma 6.2.2. □

At this stage we can finish the proof of Theorem 6.2.1.

Proof. From Lemma 6.2.3 we conclude that ψ_k's form a totally isotropic subspace with respect to Hermitian form $A \otimes I_d$ of dimension td. Lemma 6.1.2 establishes the upper bound on dimension of such subspace as $n^0(A \otimes I_d) + \min\{n^+(A \otimes I_d), n^-(A \otimes I_d)\}$. Since eigenvalues of tensor product are products of eigenvalues of corresponding matrices, and all eigenvalues of I_d are 1, we simplify the expression to:

$$td \leq d(n^0(A) + \min\{n^+(A), n^-(A)\})$$
$$\alpha_q = t \leq n^0(A) + \min\{n^+(A), n^-(A)\},$$

establishing the quantum inertia bound. □

After considering the inertia bound above, we will get familiar with one more graph parameter, which is an upper bound for both α and α_q. This is the well-known Lovász theta.

6.3 Lovász theta and inertia bound

The inertia bound and Lovász theta are not comparable. We will provide an example of a strongly regular graph, the Clebsch graph, to support this claim. Theorem 9 in the seminal Lovász paper [16] states the following.

6.3.1 Theorem. *Let G be a regular graph, and let $\lambda_1 \geq \lambda_2 \geq ... \geq \lambda_n$ be the eigenvalues of its adjacency matrix A. Then*

$$\vartheta(G) \leq \frac{-n\lambda_n}{\lambda_1 - \lambda_n}.$$

Equality holds if the automorphism group of G is transitive on the edges.

It is known that the Clebsch graph X is edge transitive and thus the application of the previous theorem shows that its $\vartheta(X) = 6$. The simple calculation shows that its inertia bound is five, coinciding with the independence number.

On the other hand, consider a cycle graph on six vertices, C_6. This graph is also edge transitive, so $\vartheta(C_6) = 2$. However, in this graph the inertia bound is three.

When one bound is not tight, another one could provide a better insight in proving that α and α_q are the same for a particular graph. Using this strategy, we will see immediately that both bipartite and perfect graphs do not exhibit quantum versus classical coclique number separation. Lovász's ϑ was also helpful to show that Paley graph on 13 vertices has no separation, for which it is not known whether the inertia bound is tight [28]. With a bit more work in the other section, we will prove the same statement for G_{13}, the graph from the [20] paper.

6.4 Direct proof of $\alpha_q(G) \leq \vartheta(G)$

By 2013 it was known that Lovász theta is an upper bound for $\alpha_q(G)$ - Scarpa mentioned the bound in his thesis [27]. There was no direct proof, but a chain of results, for example, from Beigi [5] and Piovesan [23] implied the bound. In the appendix we state those theorems, but in the main section, we will prove the bound directly. It is a simplified version of Beigi's proof. First, we will provide the definition of ϑ, that is found in [16] and is used by Beigi [5].

Definition (Lovász theta)**.**

$$\begin{aligned} \vartheta(G) = & \max \operatorname{tr}(BJ) \\ B & \succeq 0 \\ \operatorname{tr} B & = 1 \\ B_{uv} & = 0 \text{ for every edge } uv \in E(G). \end{aligned}$$

6.4.1 Theorem ([5],[10],[23])**.** *For any graph G, we have that $\alpha_q(G) \leq \vartheta(G)$.*

Below is our short adaptation of the Beigi's proof.

Proof. Suppose, $\alpha_q(G) = k$. Then there are $d \times d$ projections $\{P^{(u,i)}\}_{u \in V(G), i \in [k]}$ satisfying the following conditions.

(1) $\sum_u P^{(u,i)} = I_d$ for all $i \in [k]$

(2) $\langle P^{(u,i)}, P^{(v,i)} \rangle = 0$ for every $u \neq v \in E(G)$

(3) $\langle P^{(u,i)}, P^{(v,j)} \rangle = 0$ for every edge $uv \in E(G)$

(4) $\langle P^{(u,i)}, P^{(u,j)} \rangle = 0$ for every $i \neq j \in E(G)$

Now, define a $|V(G)| \times |V(G)|$ matrix B, such that $B_{uv} = \langle P_u, P_v \rangle$, where $P_u = \sum_i P^{(u,i)}$. We will show that matrix

$$\frac{B}{\operatorname{tr} B}$$

satisfies the conditions of the ϑ program 6.4 so

$$\vartheta \geq \frac{\operatorname{tr} BJ}{\operatorname{tr} B},$$

which will turn out to be $\alpha_q(G)$.
<u>Claim:</u> Matrix B is positive semidefinite.
<u>Proof:</u> Suppose we have two $d \times d$ Hermitian matrices $S = S^*$ and $R = R^*$. Label rows of S as $s_1, ..., s_n$ and rows of R as $r_1, ..., r_n$. Then their inner product is

$$\langle S, R \rangle = \operatorname{tr} S^* R = \sum_{i \in [d]} \langle s_i, r_i \rangle.$$

Now, our matrix B resembles a Gram matrix, since its entries are inner products of the vectors in matrix Hilbert space $\langle P_u, P_v \rangle$ for $u, v \in V(G)$. We will define a matrix M such that $B = MM^*$, to prove that B is positive semidefinite.

Let M be a $n \times d$ block matrix with $(u, j)^{th}$ block being the j^{th} row of P_u. By u_i denote the i^{th} row of P_u and observe that

$$(MM^*)_{u,v} = \sum_{i \in [d]} \langle u_i, v_i \rangle = \operatorname{tr} P_u P_v = \operatorname{tr} P_u^* P_v = \langle P_u, P_v \rangle = B_{u,v}.$$

$\blacksquare$

Claim: $\operatorname{tr} B = \alpha_q d = kd$.
Proof:

$$\operatorname{tr} B = \sum_{u \in V(G)} \langle P_u, P_u \rangle = \sum_{u \in V(G)} \langle P^{(u,1)} + ... + P^{(u,k)}, P^{(u,1)} + ... + P^{(v,k)} \rangle.$$

From the orthogonality relations, $\langle P^{(u,i)}, P^{(u,j)} \rangle = 0$ for any $i \neq j$. Thus, we have

$$\operatorname{tr} B = \sum_{u \in V(G)} \sum_{i \in [k]} \langle P^{(u,i)}, P^{(u,i)} \rangle = \sum_{i \in [k]} \sum_{u \in V(G)} \langle P^{(u,i)}, P^{(u,i)} \rangle = \sum_{i \in [k]} \langle I_d, I_d \rangle = kd.$$

$\blacksquare$

Claim: $\operatorname{tr} BJ = \alpha_q^2 d = k^2 d$.
Proof: First, consider the i^{th} diagonal entry $BJ_{i,i}$.

$$BJ_{i,i} = \sum_{v \in V(G)} \langle P_u, P_v \rangle = \sum_{v \in V(G)} \sum_{i,j} \langle P^{(u,i)}, P^{(v,j)} \rangle.$$

Hence,

$$\operatorname{tr} BJ = \sum_{v \in V(G)} \langle P_u, P_v \rangle = \sum_{u,v \in V(G)} \sum_{i,j} \langle P^{(u,i)}, P^{(v,j)} \rangle.$$

Rewriting ths sum as

$$\sum_{i \in [k]} \langle P^{(v_1,i)} + ... + P^{(v_n,i)}, P^{(v_1,j)} + ... + P^{(v_n,j)} \rangle = \sum_{i,j \in [k]} \langle I_d, I_d \rangle = k^2 d.$$

$\blacksquare$

Now, we have confirmed that $\alpha_q = \frac{\operatorname{tr} BJ}{\operatorname{tr} B}$, which was enough to prove the theorem. $\square$

6.5 Appendix

We will fist define a new quantity, and explain below how it relates to the $\alpha_q \leq \vartheta(G)$ inequality.

Definition. Denote by $\alpha^*(G)$ the maximum number m for which there exist POVMs $\{P_u^i\}_{i\in[m]}$, and $\{Q_j^{uv}\}_{j\in[m]}$ for every edge uv of G such that for some fixed bipartite state $|\psi\rangle$ we have

$$\langle\psi|P_u^i \otimes Q_j^{uv}|\psi\rangle = \delta_{ij}.$$

Beigi in Theorem 1 of [5] proves that

$$\vartheta(G) \geq \alpha^*(G).$$

Then Piovesan in Corollary 5.1.17 proves that

$$\alpha_q(G) \leq \alpha^*(G).$$

Together these two results imply that $\alpha_q(G) \leq \vartheta(G)$. However, the proof of the above mentioned Beigi's Theorem 1 is essentially the proof that $\alpha_q(G) \leq \vartheta(G)$. For our purposes, the ordinary matrix trace norm was enough, so we did not define a specific matrix norm as in the proof. The reasoning about positive semidefiniteness was different as well.

Chapter 7

Open questions

While working in this fascinating topic, we have studied a lot of existent literature and were able to answer some questions and to identify new ones.

We started by reviewing and confirming the bound on chromatic number derived from the orthogonal representation in dimensions between three and eight from [7]. The construction relies on the properties of the only finite division algebras in this dimension range, the quaternions and octonions. This bound is extremely useful and has been the key tool for coming up with the graphs exhibiting the chromatic numbers gap. We would like to know if there are bounds in higher dimensions of orthogonal representations, and possibly for independence numbers as well.

In the same chapter we proved results that are accordant with the classical expectations. The more we know about the cases when the quantum and classical quantities coincide, the more restrictive is the search for the cases when they differ. For this reason, we are hoping to see progress in the future involving bounds that are either bounding both the classical and the quantum parameter, or are squeezed between the two parameters.

Searching for graphs with the classical versus quantum chromatic number gap, we were able to generalise Mančinska and Roberson's example [20] to an infinite family. One way to further the research would be to look for more infinite families with the separation.

As the separations are one of the purposes of this work, we have studied the three main examples of the difference between the quantum and classical independence numbers. We have successfully found a new Cayley representation for the Piovesan's example [23, Page 34], which helped us find a new graph with the separation. Scarpa characterised chromatic numbers separation in terms of projective Kochen-Specker sets and showed how to obtain a graph with the independence numbers separation given a graph with the gap between the chromatic numbers. We related Projective Kochen-Specker sets further with the separation between the independence numbers, which has provided another link between the quantum chromatic number and the quantum independence number. It would be interesting to know how else the two parameters relate.

1 Question. Can we find a graph X with $\chi(X) > \chi_q(X)$ if we have a graph G such that $\alpha(G) < \alpha_q(G)$? How else can one relate χ_q and α_q?

So far the prevalent majority of examples, including the one we found, has been coming from the orthogonal representations and have only rank-1 projections. This leaves a question of finding more versatile examples with the quantum and classical separations, as well as learning more about the rank-one quantum graph parameters in comparison with the general ones.

2 Question. Find a graph G such that $\chi_q(G) < \chi(G)$. What is the smallest such graph? What are the new infinite families $\mathcal{F}$ such that for every $G \in \mathcal{F}$ we have $\chi_q(G) < \chi(G)$?

3 Question. Find a graph G such that $\alpha_q(G) > \alpha(G)$. What is the smallest such graph? What are the new infinite families $\mathcal{F}$ such that for every $G \in \mathcal{F}$ we have $\alpha_q(G) > \alpha(G)$?

This brings a related question of what role does the dimension of the projections in the definition of either the quantum chromatic or quantum independence number play?

4 Question. Is there a graph G such that $\chi_q^{(c)}(G) \neq \chi_q^{(d)}(G)$, where $c, d > 1$? and $c \neq d$? With the same restrictions, can it happen that $\alpha_q^{(c)}(X) \neq \alpha_q^{(d)}(X)$ for some graph X?

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