Bell Monogamy

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Abstract

A single Bell's inequality is violated by quantum predictions and demonstrates impossibility of classical-like model beyond quantum statistics. Interestingly, several Bell inequalities often cannot be violated simultaneously–a fact known as Bell monogamy. In this thesis we will formulate a method within graph theory to obtain the Bell monogamy relations from no-signalling principle. We also borrowed the derivation used to obtain the entropic uncertainty relation to re-derive the bound on Bell monogamy relation using the correlation complementarity principle. It is shown that a tighter bound could in principle be obtained using this new derivation. We introduce the notion of elementary monogamy relations and solve completely their existence for bipartite Bell inequalities. We obtain three elementary tripartite Bell monogamy relations from the complementarity principle and we conjecture that there is no finite set of elementary Bell monogamy relations in the multipartite case.

Acknowledgements

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Last but not least, I would like to delicate this thesis to my parents for their unconditional love and support throughout my life. I also want to thank my sisters for their encouragement and support whenever I needed them.

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Contents

Chapter 1

Introduction

Looking at the equations of quantum mechanics, the world we live in indeed seems bizarre. Quantum mechanics was introduced to explain conundrums in classical physics such as the blackbody radiation, photoelectric effect and electron orbital stability, and the basic foundation of quantum mechanics was in placed in the 1930s. It remains undoubtedly one of the most accurate descriptions of the natural world. However, we hardly have any intuition in quantum mechanics, probably because our classical notion of local reality is not build in quantum mechanics. Even Albert Einstein had his various tensions with this paradigm shift[1]. In 1964, a Northern Irish physicist John Bell published an important no-go theorem in quantum mechanics, the Bell's theorem[2], which challenged the concept of local realism handed down by Galileo and Newton. It was found that Bell inequalities are monogamous[3], but the guiding principle for the monogamy still remains unknown. In this thesis we will explore the Bell's theorem and derive Bell monogamy relations from various general principles.

In Chapter 2, we review the Bell's theorem which shows that quantum mechanics cannot be explained by any local hidden variable theories. Then, in Chapter 3, we will introduce the concept of Bell monogamy, and look at some fundamental principles and methods to obtain the Bell monogamy relations, namely the no-signalling principle, Schmidt decomposition method, and complementarity principle.

We present a graph theoretic method to obtain the bound from no-signalling principle for any arbitrary systems. Next we show that Schmidt decomposition can be used to obtain Bell monogamy relations. After that we re-derive the result from complementarity principle to obtain Bell monogamy relations using the method in [4]. Obtaining the Bell monogamy relation from complementarity is equivalent to solving for the clique covering number of the complementarity graph, which is a NP-complete problem, and we will provide an algorithm to attempt to solve it. We show that by averaging the elementary relations we can compute the Bell monogamy relations more quickly, although the efficiency is still limited as the problem is still NP-complete.

In Chapter 4, we focus on the complementarity principle to obtain tight Bell monogamy relations. We first review the bipartite Bell monogamy relations and introduced the notion of elementary monogamy relation. We then extend it to tripartite monogamy relations. We also provided a recipe to construct a group of elementary Bell monogamy relations for k-partite relations, which we call the frankenstein graphs. Finally, we conjecture that the complementarity principle alone is insufficient to obtain tight Bell monogamy relations and we have potential candidates (M-cycle graph) to affirm our belief.

Chapter 2

Bell's Theorem and Bell Monogamy

Quantum entanglement is one of the most bizarre features predicted by quantum mechanics. With entanglement it is possible to produce correlations that are stronger than intuitively possible. Einstein, Podolsky and Rosen picked up on this and published the celebrated paper in 1935 to show that quantum entanglement leads to a paradox, commonly known as the EPR paradox[1]. Because of the apparent internal inconsistency, the authors believe that quantum mechanics is an incomplete theory. The EPR argument is included in Appendix (A) for completeness.

In 1964, Bell provided a possible way to resolve the EPR paradox experimentally[2]. He formulated the Bell's inequality and show that all physical theory of local hidden variables (LHV) must obey this inequality while quantum mechanics is able to violate. In essence, Bell's theorem asserts that no physical theory of LHV can replicate all the predictions of quantum mechanics. This has serious implication as it implies that if the EPR argument is right, then quantum mechanics is wrong (and not just incomplete)[5].

Since then many experiments were conducted to investigate this theorem[6, 7, 8, 9, 10, 11, 12]. Despite having experimental loopholes, these experiments demonstrated violation of different variant of Bell's inequalities, which confirm that nature is fundamentally nonlocal.

In the later sections, we will look at what is a LHV theory and review one of the more common variant of Bell's inequalities, the Clauser-Horne-Shimony-Holt (CHSH) inequality[13]. We will also give a brief introduction to Bell monogamy relations.

2.1 Setting the Scene

A typical Bell-type experiment consists of two spatially separated observers, Alice and Bob. Each of them receives a part of a quantum system, performs a few measurements on their subsystem and obtains some measurement outcomes. After obtaining these measurement outcomes, Alice and Bob come together to calculate some Bell's inequalities to see whether they succeeded in violating the inequalities.

Throughout this thesis we will assume that there are two measurement settings for each observer and for every measurement setting there are two possible outcomes, otherwise stated. We will denote the measurement settings in capital–$\{A_1, A_2\}$ and $\{B_1, B_2\}$–and the measurement outcomes for each measurement setting in small–$\{a_1, a_2\}$ and $\{b_1, b_2\}$. The possible measurement outcomes are only ± 1. This scenario is shown in the Figure (2.1) below.

There is a probability distribution for each pair of measurement outcomes given the pair of measurement settings. This is written as:

$$p(a_j, b_k | A_j, B_k). \tag{2.1}$$

There are a few reasonable assumptions we can make about these experimental set-up which we can use to simplify the probability distribution.

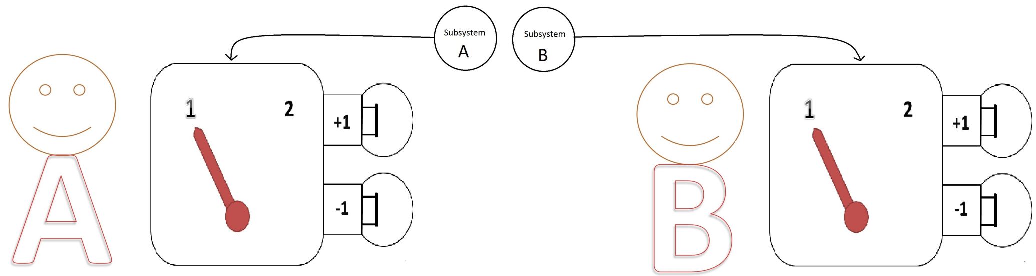


Figure 2.1: Alice on the left and Bob on the right receive subsystem A and B respectively. Each of them is able to choose freely one of the two independent measurement settings as indicated by the red arrow. There are two possible measurement outcome as indicated by the bulbs.

Assumption 1: *Free will of measurement* – The measurement settings chosen by Alice and Bob are of their free will.

This means that the measurement settings chosen are not influenced by any external forces. This can be stated mathematically as:

$$p(X|Y) = p(X), \tag{2.2}$$

where X is the setting chosen by party X and Y is the setting chosen by party Y.

Assumption 2: *Locality* – The outcome of measurements of one party is independent of the measurement settings and measurement outcomes of another party.

Assumption 2 means that measurement outcomes cannot influence each other if they are spacelike separated. In other words, measurement outcomes are independent from any action at a distant. At first sight, this assumption seems like a restatement of the principle of causality. However, it is possible to have nonlocal phenomena while preserving causality because no information is transmitted, i.e. quantum entanglement shows nonlocal effects but these effects do not transmit information. Mathematically this condition can be expressed as

$$p(a_j|A_j, B_k, b_k) = p(a_j|A_j), \tag{2.3a}$$

$$p(b_k|B_k, A_j, a_j) = p(b_k|B_k). \tag{2.3b}$$

Assumption 3: *Realism* – It refers to the simultaneous existence (i.e. well defined values) of outcomes of all possible observables(even for those which cannot be measured simultaneously).

Assumption 3 is part of a philosophical debate on whether consciousness causes a collapse of wavefunction. In this thesis, we will assume that the world is mind-independent, and the outcomes of those measurements that were not made are as real as those that were made, even if those outcomes can only be determined after the measurements.

With these three assumptions we can make useful predictions on the strength of correlation displayed by nature. Quantum correlations are stronger than classical correlations, and this is usually shown through the violation of Bell's inequalities and the non-contextual inequalities. In this thesis we will only focus on Bell's theorem and we will include quantum contextuality in appendix (B) for completeness.

2.2 Bell-CHSH Inequality

Bell-CHSH is one of the more common variants of Bell's inequality. The Bell-CHSH parameter $\mathcal{B}$ is defined to be

$$\mathcal{B} = E(A_1, B_1) - E(A_1, B_2) + E(A_2, B_1) + E(A_2, B_2), \tag{2.4}$$

where $E(A_j, B_k)$ is defined to be the expectation value of the product of measurement outcomes $\{a_j, b_k\}$, also known as the correlation function.

We will look at the bound of this particular inequality for the three different assumptions–LHV theory, quantum mechanics, and no-signalling principle.

An LHV theory assumes that nature can be explained by a local theory with some hidden variables; the randomness in quantum mechanics is attributed to the randomness of the hidden variables. Hence the probability distribution for $p(a_j, b_k|A_j, B_k)$ is given by:

$$\begin{aligned} p(a_j, b_k|A_j, B_k) &= \sum_\lambda p(a_j, b_k, \lambda|A_j, B_k) \\ &= \sum_\lambda p(\lambda|A_j, B_k) p(a_j, b_k|A_j, B_k, \lambda) \\ &= \sum_\lambda p(\lambda) p(a_j, b_k|A_j, B_k, \lambda), \end{aligned} \tag{2.5}$$

where λ is a set of hidden variables. From the second to the last step, we used the assumption of free will to simplify the probability of the hidden variables given the local measurement settings.

Furthermore, using the assumption on locality we can further simplify the probability distribution

$$p(a_j, b_k|A_j, B_k) = \sum_\lambda p(\lambda) p(a_j|A_j, \lambda) p(b_k|B_k, \lambda). \tag{2.6}$$

Fine published an important result on the condition of probability distribution of a LHV model[14]. A short proof is provided in Appendix (D).

Theorem 2.2.1. *An LHV model exist if and only if there exist a joint probability distribution for the outcomes of all possible measurement settings.*

This joint probability must return the correct marginals for all possible physical set-ups,

$$p(a_j, b_k|A_j, B_k) = \sum_{a_x|x\neq j, b_y|y\neq k} p(a_1, a_2, b_1, b_2|A_1, A_2, B_1, B_2). \tag{2.7}$$

With all these conditions on the probability distribution, the Bell-CHSH parameter is found to be bounded by $\mathcal{B}^{LHV} \leqslant 2$. The value 2 is also known as the local realistic bound.

Quantum mechanics allows a violation of the LHV bound up to $\mathcal{B}^{QM} \leqslant 2\sqrt{2}$. This maximum value is also known as the Tsirelson's bound[15]. Although we know the value of the quantum mechanical bound, we do not know what the guiding principles to obtain the bound are.

No-signalling principle is a natural principle to consider to deriving the bound on the Bell parameter as it seems like a restatement of the causality principle. In mathematical terms, it states that the measurement outcomes of one party are not influenced by the measurement settings of another spacelike separated party:

$$p(a_j|A_j, B_k) = p(a_j|A_j), \tag{2.8}$$

$$p(b_k|A_j, B_k) = p(b_k|B_k). \tag{2.9}$$

However, the bound derived from the no-signalling principle violates the quantum mechanical bound up to $\mathcal{B}^{NS} \leqslant 4$[16]. It was later found that no-signalling principle is an instance of information causality[17].

A brief derivation of the bound by various models is provided in Appendix (C).

2.3 Explaining Bell Monogamy

In our previous discussions, there are only two observers (Alice and Bob) trying to violate the local realistic bound of some Bell's inequality. We now consider a third observer. This third observer tries to violate the same type of Bell's inequality with Alice. We will call this observer Bob-two and the original Bob as Bob-one. This can be represented by the graph in Figure (2.2).

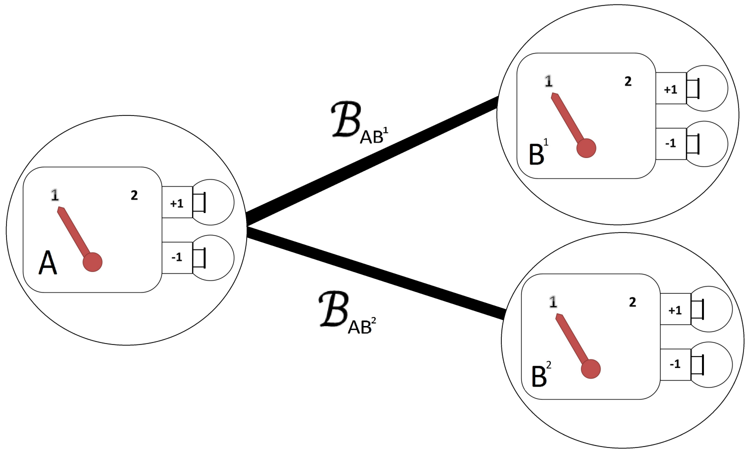


Figure 2.2: Alice on the left and two Bobs on the right. As before, each of them is able to choose freely one of the two independent measurement settings and there are two possible measurement outcomes as indicated by the bulbs. The thick black line represents the pair of observers are trying to violate the Bell's inequality, $\mathcal{B}_{AB^1}$ and $\mathcal{B}_{AB^2}$. Usually we will not include the measurement apparatus in the circles.

From [3], it was found that the two Bell parameters, $\mathcal{B}_{AB^1}$ and $\mathcal{B}_{AB^2}$, are related in quantum mechanics as

$$\mathcal{B}_{AB^1}^2 + \mathcal{B}_{AB^2}^2 \leqslant 8. \tag{2.10}$$

This equation shows that if $\mathcal{B}_{AB^1} > 2$, then $\mathcal{B}_{AB^2} < 2$; this shows a trade-off between the strength of violation of the Bell's inequalities because when one Bell parameter is allowed to violate the local realistic bound, the other one cannot violate the local realistic bound. The trade-off between the maximum values of the Bell parameters is called Bell monogamy relation. We can also see that the Tsirelson's bound is a collorary of equation (2.10) as we can set one of terms to zero to obtain the bound.

A weaker monogamy relation from the no-signalling principle is obtained in [18] as

$$\mathcal{B}_{AB^1} + \mathcal{B}_{AB^2} \leqslant 4, \tag{2.11}$$

and the equations for LHV theories are

$$\begin{aligned} \mathcal{B}_{AB^1} &\leqslant 2, \\ \mathcal{B}_{AB^2} &\leqslant 2. \end{aligned} \tag{2.12}$$

A graph is plotted in Figure (2.3) to show the differences between the bound obtained from LHV theories, quantum mechanics, and no-signalling principle.

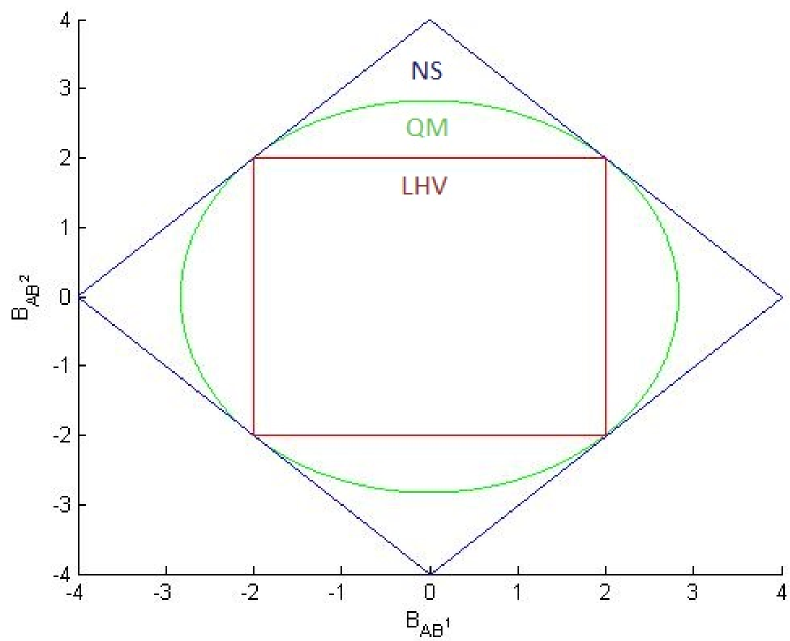


Figure 2.3: The region within the blue line is the bound obtained from the no-signalling (NS) principle, the green line is the bound obtained from quantum mechanics, and the red line is the bound obtained from LHV theories.

Before proceeding to the next chapter, we will introduce some terms that will be used throughout the thesis.

The Bell monogamy relation is called *bipartite* if there are only two-observers involved in each Bell parameter. So far we have only looked at bipartite monogamy relations. Bipartite monogamy relations can be represented by *bipartite graphs* like in Figure (2.2). A vertex (a dot) in the bipartite graph represents an observer and an edge (a line) between two vertices, say Alice and Bob, represents the Bell parameter $\mathcal{B}_{AB}$.

Likewise a *k-partite* relation is if there are k-observers involved in each Bell parameter. k-partite relations can be represented by a hypergraph called the *k-partite graph*; the vertices represent the observers, and the hyperedges represent the Bell parameters for the k observers in it. An example of a *tripartite graph* is shown in Figure (2.4).

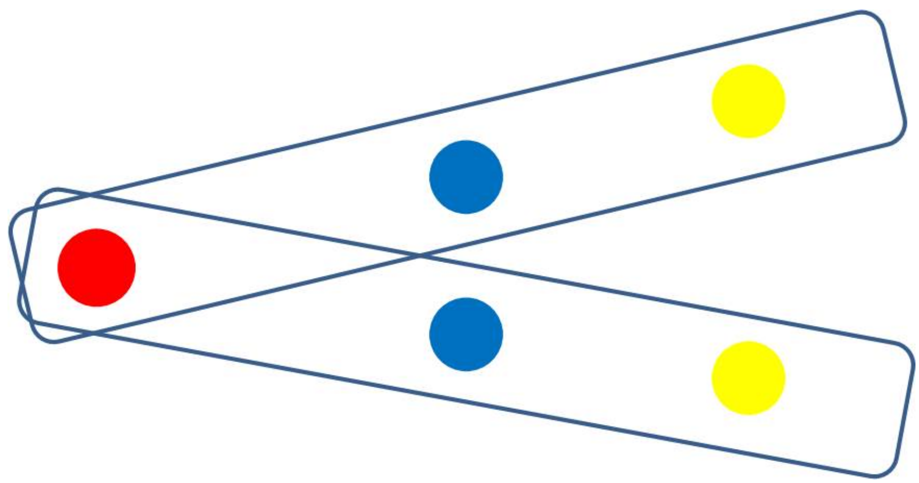


Figure 2.4: A hypergraph showing tripartite monogamy relation.

In the next section, we will look at some general principles to obtain the Bell monogamy relations.

Chapter 3

Principles and Methods to obtain Bell Monogamy relation

3.1 No-signalling Principle

No-signalling principle plays a special role in quantum mechanics. It implies many no-go theorems, i.e. no-cloning theorem and no-broadcasting theorem[19, 20], and their corollary, the no-deleting theorem.

The no-signalling principle can be used to derive the bound for Bell monogamy relations. We identified a fault in [21] for deriving the bound for multipartite monogamy relations, and we will present an alternative approach to obtain the Bell monogamy relations and formulate it as a problem in graph theory.

We will look at bipartite Bell monogamy relations first. Any bipartite Bell parameter can be expressed as

$$\mathcal{B}_{A,B^i} = \sum_{j,k=1}^{2} \sum_{a,b=\pm 1} \alpha(j,k,a,b) p(a_j = a, b_k^i = b | A_j, B_k^i), \tag{3.1}$$

where $\alpha(j,k,a,b)$ is any arbitrary function. This Bell parameter has a local realistic bound R. For example in Bell-CHSH parameter in equation (2.4), $\alpha(j,k,a,b) = ab$ for

$\{j, k\} = \{1, 1\}, \{2, 1\}, \{2, 2\}$ and $\alpha(j = 1, k = 2, a, b) = -ab$, and the local realistic bound is 2.

Consider the case where the monogamy relation is between Alice and two Bobs. The Bell parameter for Alice and Bob-one is denoted by $\mathcal{B}_{AB^1}$ and for Alice and Bob-two is denoted by $\mathcal{B}_{AB^2}$. Adding the two Bell parameters together and rearranging the terms,

$$\begin{aligned}
\mathcal{B}_{AB^1} + \mathcal{B}_{AB^2} = &\sum_{a,b} \Big[\alpha(1,1)p(a_1, b_1^1) + \alpha(1,2)p(a_1, b_2^1) + \alpha(2,1)p(a_2, b_1^1) + \alpha(2,2)p(a_2, b_2^1) \\
&+ \alpha(1,1)p(a_1, b_1^2) + \alpha(1,2)p(a_1, b_2^2) + \alpha(2,1)p(a_2, b_1^2) + \alpha(2,2)p(a_2, b_2^2)\Big] \\
&= \sum_{a,b} \Big\{ \big[\alpha(1,1)p(a_1, b_1^1) + \alpha(1,2)p(a_1, b_2^2) + \alpha(2,1)p(a_2, b_1^1) + \alpha(2,2)p(a_2, b_2^2)\big] \\
&+ \big[\alpha(1,1)p(a_1, b_1^2) + \alpha(1,2)p(a_1, b_2^1) + \alpha(2,1)p(a_2, b_1^2) + \alpha(2,2)p(a_2, b_2^1)\big]\Big\} \\
&= \mathcal{B}^1 + \mathcal{B}^2,
\end{aligned} \tag{3.2}$$

where we have made the equation more readable by writing $\alpha(j, k, a, b) \equiv \alpha(j, k)$ and $p(a_j = a, b_k^i = b|A_j, B_k^i) \equiv p(a_j, b_k^i)$, and

$$\begin{aligned}
\mathcal{B}^1 &\equiv \alpha(1,1)p(a_1, b_1^1) + \alpha(1,2)p(a_1, b_2^2) + \alpha(2,1)p(a_2, b_1^1) + \alpha(2,2)p(a_2, b_2^2), \\
\mathcal{B}^2 &\equiv \alpha(1,1)p(a_1, b_1^2) + \alpha(1,2)p(a_1, b_2^1) + \alpha(2,1)p(a_2, b_1^2) + \alpha(2,2)p(a_2, b_2^1).
\end{aligned}$$

Note that the coefficients for the probabilities, $\alpha(j, k)$, in $\mathcal{B}^1$ and $\mathcal{B}^2$ have the same structure as the Bell parameter. It is, hence, possible to construct a joint probability distribution

$$p(a_1, a_2, b_1^1, b_2^2) = \frac{p(a_1, b_1^1, b_2^2)p(a_2, b_1^1, b_2^2)}{p(b_1^1, b_2^2)}, \tag{3.3a}$$

$$p(a_1, a_2, b_2^1, b_1^2) = \frac{p(a_1, b_1^2, b_2^1)p(a_2, b_1^2, b_2^1)}{p(b_1^2, b_2^1)}, \tag{3.3b}$$

where the probabilities $p(a_1, b_1^1, b_2^2)$, $p(a_2, b_1^1, b_2^2)$, $p(a_1, b_1^2, b_2^1)$ and $p(a_2, b_1^2, b_2^1)$ exist because the measurements are done by different observers. This joint probability distribution returns all the necessary marginal probabilities because of the no-signalling principle

$$\sum_{a_1} p(a_1, b_1^1, b_2^2) = p(b_1^1, b_2^2) = \sum_{a_2} p(a_2, b_1^1, b_2^2), \tag{3.4}$$

$$\sum_{a_1} p(a_1, b_1^2, b_2^1) = p(b_1^2, b_2^1) = \sum_{a_2} p(a_2, b_1^2, b_2^1). \tag{3.5}$$

Therefore, by Theorem 2.2.1, $\mathcal{B}^1 \leqslant R$ and $\mathcal{B}^2 \leqslant R$. Hence we obtain the monogamy relation as in equation (2.11),

$$\mathcal{B}_{AB^1} + \mathcal{B}_{AB^2} = \mathcal{B}^1 + \mathcal{B}^2 \leqslant 2R. \tag{3.6}$$

The concept behind this derivation of monogamy relations is to arrange the terms of the Bell parameters into as little groups as possible, such that it is possible to construct a valid joint probability distribution for each group using the no-signalling principle. Each group must have similar structure as the original Bell parameters so that the groups are bounded by the local realistic bound. Using this concept we will construct a method to obtain the bound on the monogamy relation for k-partite systems.

Before proceeding, we will briefly introduce two terms in graph theory, *clique* and *chromatic number*. A clique is a graph where all its vertices are adjacent to each other. Chromatic number of a graph is the minimum number of colours needed to paint the vertices such that no adjacent vertices have the same colour.

We will use the monogamy of $\mathcal{B}_{AB^1C^1}$ and $\mathcal{B}_{AB^2C^2}$ shown in Figure (2.4) as a walkthrough of this construction. We separate the observers into two sets, the common observers (CO) set and the not common observers (NCO) set. The red dot in Figure

(2.4) represents observer A the CO, and the two blue and two yellow dots represent observers B^1, B^2, C^1 and C^2 respectively, and they are the NCO.

In the NCO set, represent the measurement settings from every possible observation combinations as a vertex. Connect the vertices with an edge if they are from the same observers, or if they have the same combination of measurement settings. After constructing this NCO graph, evaluate its chromatic number χ^{NCO}. The NCO graph for the walkthrough example is shown in Figure (3.1).

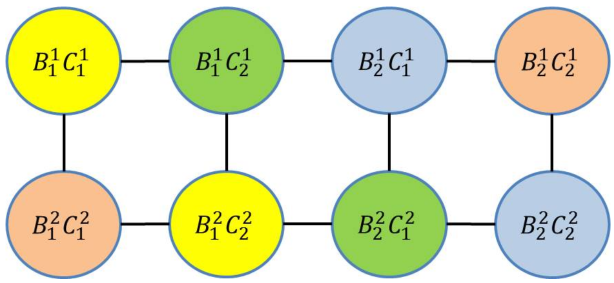


Figure 3.1: This graph shows the NCO graph for the monogamy of $\mathcal{B}_{AB^1C^1}$ and $\mathcal{B}_{AB^2C^2}$. Every vertex represents a measurement setting in the NCO set. Vertices in a row are from the same observers, and vertices in a column have the same combination of measurement settings. Hence, vertices lined up in a row or a column form a clique. The chromatic number of this graph is $\chi^{NCO} = 4$.

In the CO set, represent every possible measurement settings as a vertex. Connect the vertices with an edge if they have at least one observer with the same setting. After constructing this CO graph, again, evaluate its chromatic number χ^{CO}. The CO graph for the walkthrough example is shown in Figure (3.2).

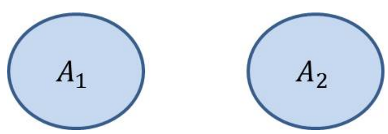


Figure 3.2: This graph shows the CO graph for the monogamy of $\mathcal{B}_{AB^1C^1}$ and $\mathcal{B}_{AB^2C^2}$. Every vertex represents a measurement setting in the CO set. Connect vertices with at least one observer having the measurement setting with an edge. In this example there are no measurement settings with the same observer measuring the same measurement setting. The chromatic number $\chi^{CO} = 1$.

After evaluating χ^{NCO} and χ^{CO}, multiply them together to obtain the bound on the monogamy relation.

We construct the graphs in this way because it ensures that it is possible to construct a joint probability distribution.

Referring to the walkthrough example, the vertices with the same colour in the NCO graph, for instance yellow colour, ensure that the probability $p(b_1^1, c_1^1, b_1^2, c_2^2)$ exist and is consistent with the structure of the Bell parameter. The vertices with the same colour in the CO graph ensure that we can construct a valid joint probability like in equation (3.3). Therefore the joint probability can be constructed in this manner:

$$p(a_1, a_2, b_1^1, c_1^1, b_1^2, c_2^2) = \frac{p(a_1, b_1^1, c_1^1, b_1^2, c_2^2)p(a_2, b_1^1, c_1^1, b_1^2, c_2^2)}{p(b_1^1, c_1^1, b_1^2, c_2^2)}. \tag{3.7}$$

We multiply the chromatic numbers together because every colour in the CO graph can be combined together with every colour group in the NCO graph to form a valid joint probability distribution. Hence the monogamy relation from the no-signalling principle for the walkthrough example is

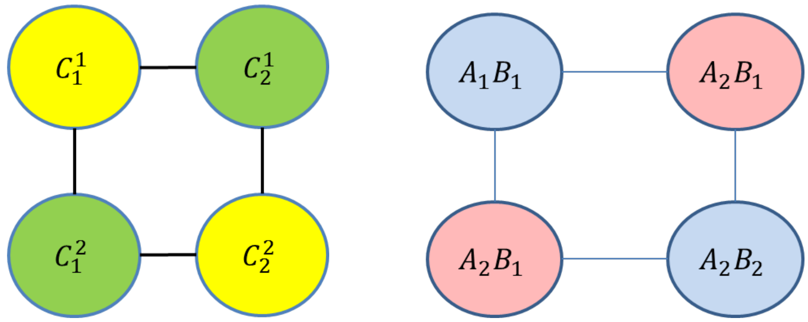
$$\mathcal{B}_{AB^1C^1} + \mathcal{B}_{AB^2C^2} \leqslant 4R. \tag{3.8}$$

We will provide another example to make the processes clearer. We will look at the monogamy of $\mathcal{B}_{ABC^1}$ and $\mathcal{B}_{ABC^2}$. The NCO set consists of observers $\{C^1, C^2\}$ and the CO set consists of observers $\{A, B\}$.

The NCO graph is in Figure (3.3a) and $\chi^{NCO} = 2$. The CO graph is in Figure (3.3b) and $\chi^{CO} = 2$.

We are able to construct the joint probability distribution for, say, the yellow and blue groups

$$p(a_1, b_1, a_2, b_2, c_1^1, c_2^2) = \frac{p(a_1, b_1, c_1^1, c_2^2)p(a_2, b_2, c_1^1, c_2^2)}{p(c_1^1, c_2^2)}. \tag{3.9}$$



(a) The NCO graph. The chromatic number $\chi^{NCO} = 2$.

(b) The CO graph. The chromatic number $\chi^{CO} = 2$.

Figure 3.3: Monogamy relation for $\mathcal{B}_{ABC^1}$ and $\mathcal{B}_{ABC^2}$.

Hence it is bounded by the local realistic bound R. Likewise for every other combination of colours of the NCO and CO graphs. Therefore the no-signalling bound for the monogamy relation is

$$\mathcal{B}_{ABC^1} + \mathcal{B}_{ABC^2} \leqslant \chi^{NCO}\chi^{CO} \times R = 4R. \tag{3.10}$$

We would like to give some remarks on our method to derive Bell monogamy relations from no-signalling principle. Our method reduces to the same result in [21] for bipartite monogamy when we take the same assumption as in the paper (the number of Bobs must be greater than or equals to the number of settings of each Bob). Furthermore, we would like to clarify that the bound for multipartite case in the paper is incorrect and it is not $\sum_{m=1}^{n} \mathcal{B}_{\vec{A},\vec{B}^m} \leqslant nR$, where $\vec{A}$ are the common observers, $\vec{B}^m$ are the non-common observers for the m^{th} Bell parameter, and n is the number of settings for each $\vec{B}^m$. This can be seen from the last example of this section where the bound from the result of the paper is $2R$, in contrast to equation (3.10). The reason for this error is that no-signalling between individual observers cannot be assumed in the multipartite case.

3.2 Schmidt decomposition

In this section, we will demonstrate how Schmidt decomposition can be used to obtain simple Bell monogamy relations of a composite system. We will show this by an example of a 3-qubit system.

Schmidt decomposition is a mathematical theorem that expresses a vector as the tensor product of two inner product spaces. Formally the theorem states that for any vector $|\psi\rangle \in H_1 \otimes H_2$ where $\{|v_1\rangle, ..., |v_n\rangle\} \subset H_1$ and $\{|w_1\rangle, ..., |w_m\rangle\} \subset H_2$ are Hilbert spaces of dimensions n and m, $n \leqslant m$, and $\langle v_j|v_k\rangle = \delta_{jk}$ and $\langle w_j|w_k\rangle = \delta_{jk}$, $|\psi\rangle$ can be expressed as

$$|\psi\rangle = \sum_{j=1}^{n} \lambda_j |v\rangle_j \otimes |w\rangle_j , \tag{3.11}$$

where $\lambda_j \geqslant 0$.

Applying Schmidt decomposition on a 3-qubit state, we can write the state as

$$|\psi\rangle = \lambda_1 |0_1\rangle |w_{23}\rangle_1 + \lambda_2 |1_1\rangle |w_{23}\rangle_2 , \tag{3.12}$$

where $\{|0_1\rangle, |1_1\rangle\}$ are the eigenstates for the first qubit, and $|w_{23}\rangle_1$ and $|w_{23}\rangle_2$ are two orthonormal states in the combine Hilbert space of the second and third qubits. Taking the partial trace over qubit 2 and 3, the reduced density matrix is

$$\rho_1 = \lambda_1^2 |0\rangle \langle 1| + \lambda_2^2 |0\rangle \langle 1| . \tag{3.13}$$

Taking the partial trace over qubit 1, one obtains a similar reduced density matrix

$$\rho_{23} = \lambda_1^2 |w_{23}\rangle_1 \langle w_{23}|_1 + \lambda_2^2 |w_{23}\rangle_2 \langle w_{23}|_2 . \tag{3.14}$$

Taking the trace of the square of the two reduced density matrices, one obtains

$$\mathrm{tr}(\rho_1^2) = \mathrm{tr}(\rho_{23}^2) = \lambda_1^4 + \lambda_2^4. \tag{3.15}$$

In the next part of this section (and subsequent sections), we will rely on an important result from [22]. The proof of the result is in Appendix (E).

An arbitrary N-qubit state can be expressed as

$$\rho = \frac{1}{2^N} \sum_{\mu_1,\ldots,\mu_N=0}^{3} T_{\mu_1\ldots\mu_N} \sigma_{\mu_1}^1 \otimes \ldots \otimes \sigma_{\mu_N}^N, \tag{3.16}$$

where σ_0^j is the identity operator and $\sigma_{x_j}^j$ are the local Pauli operators for the three orthogonal directions $x_j = 1, 2, 3$ in the Hilbert space of the jth qubit. The set of components $T_{\mu_1\ldots\mu_N} = \mathrm{tr}(\rho.(\sigma_{\mu_1}^1 \otimes \ldots \otimes \sigma_{\mu_N}^N))$ corresponding to the three orthogonal Pauli operators forms the *correlation tensor*, $\hat{T}$. The N-qubit state admits a LHV model if the condition

$$\mathcal{B}^2 \leqslant \sum_{x_1,\ldots,x_N=1}^{2} T_{x_1\ldots x_N}^2 \leqslant 1 \tag{3.17}$$

holds for any local coordinate systems. Note that we have set the local realistic bound for the Bell parameter to 1.

Rather than using the Schmidt decomposition to represent the 3-qubit state, we can represent the state as in equation (3.16)

$$\rho = \frac{1}{8} \left(\sum_{\mu_1,\mu_2,\mu_3=0}^{3} T_{\mu_1\mu_2\mu_3} \sigma_{\mu_1}^1 \otimes \sigma_{\mu_2}^2 \otimes \sigma_{\mu_3}^3 \right). \tag{3.18}$$

Since the Pauli operators are traceless and the identity operator (of dimension 2) has trace 2, the reduced density matrix for qubit 1 is

$$\begin{aligned}\rho_1 &= \mathrm{tr}_{23}\left[\frac{1}{8}\left(\sum_{\mu_1,\mu_2,\mu_3=0}^{3} T_{\mu_1\mu_2\mu_3}\sigma^1_{\mu_1}\otimes\sigma^2_{\mu_2}\otimes\sigma^3_{\mu_3}\right)\right] \\ &= \frac{1}{2}\left(\sigma^1_0 + \sum_{j=1}^{3} T_{j00}\sigma^1_j\right).\end{aligned} \tag{3.19}$$

The reduced density matrix for qubit 2 and 3 is

$$\rho_{23} = \frac{1}{4}\left(\sigma^2_0\otimes\sigma^3_0 + \sum_{j=1}^{3} T_{0j0}\sigma^2_j\otimes\sigma^3_0 + \sum_{j=1}^{3} T_{00j}\sigma^2_0\otimes\sigma^3_j + \sum_{j,k=1}^{3} T_{jk}\sigma^2_j\otimes\sigma^3_k.\right) \tag{3.20}$$

Calculating the trace of ρ_1^2 and ρ_{23}^2 and using the property in equation (3.15),

$$\frac{1}{2}\left(1 + \sum_{j=1}^{3} T^2_{j00}\right) = \frac{1}{4}\left(1 + \sum_{j=1}^{3} T^2_{0j0} + \sum_{j=1}^{3} T^2_{00j} + \sum_{j,k=1}^{3} T^2_{0jk}\right). \tag{3.21}$$

Repeating these procedures to qubit 2 and qubit 3, one obtains the other two relations

$$\frac{1}{2}\left(1 + \sum_{j=1}^{3} T^2_{0j0}\right) = \frac{1}{4}\left(1 + \sum_{j=1}^{3} T^2_{j00} + \sum_{j=1}^{3} T^2_{00j} + \sum_{j,k=1}^{3} T^2_{j0k}\right), \tag{3.22}$$

$$\frac{1}{2}\left(1 + \sum_{j=1}^{3} T^2_{00j}\right) = \frac{1}{4}\left(1 + \sum_{j=1}^{3} T^2_{j00} + \sum_{j=1}^{3} T^2_{0j0} + \sum_{j,k=1}^{3} T^2_{jk0}\right) \tag{3.23}$$

Adding these three relations and simplifying it, one obtains the following monogamy relation:

$$\sum_{j,k=1}^{3} T^2_{jk0} + \sum_{j,k=1}^{3} T^2_{j0k} + \sum_{j,k=1}^{3} T^2_{0jk} = 3. \tag{3.24}$$

This is a monogamy relation because it relates the correlation tensor between pairs of qubits–the first term is the correlation tensor for the first and second qubits, the second term is for the first and third qubits and the last term is for the second and last qubits. The sum of the squares of the correlation tensors is 3, regardless of how we achieve it. This shows a trade-off between the values of the correlation tensors.

Note that the terms in equation (3.24) does not relate to Bell's inequality as the terms have a different form as in equation (3.17). However we can set it as an upper bound to the Bell monogamy relation,

$$\begin{aligned}\mathcal{B}_{12}^2 + \mathcal{B}_{13}^2 + \mathcal{B}_{23}^2 &\leqslant \sum_{j,k=1}^{2} T_{jk0}^2 + \sum_{j,k=1}^{2} T_{j0k}^2 + \sum_{j,k=1}^{2} T_{0jk}^2 \\ &\leqslant \sum_{j,k=1}^{3} T_{jk0}^2 + \sum_{j,k=1}^{3} T_{j0k}^2 + \sum_{j,k=1}^{3} T_{0jk}^2 \\ &= 3.\end{aligned} \tag{3.25}$$

In Section (3.3), we will show that more Bell monogamy relations are needed to describe this quantum mechanical systems of 3-qubits.

3.3 Correlation complementarity principle

Complementarity is the bedrock of the uncertainty principle in quantum mechanics. It was found in [23] that complementarity principle plays an important role in Bell monogamy relations within quantum formalism. Due to its importance, we will show how it relates to Bell monogamy relations as in the paper.

3.3.1 Bound on the Bell parameter

Theorem 3.3.1. *Within quantum formalism, any pair of complementary dichotomic observables with eigenvalues* $+1$ *and* -1 *anticommutes.*

Proof. Consider two complementary dichotomic observables $\hat{A}$ and $\hat{B}$ with eigenvalues $+1$ and -1. Let the eigenstates of $\hat{A}$ with eigenvalue $+1$ be $|a\rangle$. From complementarity, it is required that $\langle a|\,\hat{B}\,|a\rangle = 0$, which implies that $\hat{B}\,|a\rangle = |a_\perp\rangle$, where $|a_\perp\rangle$ is orthogonal to $|a\rangle$. Since $\hat{B}^2 = \mathbb{1}$, one obtains $\hat{B}\,|a_\perp\rangle = |a\rangle$. Hence, $|b\rangle = \frac{1}{\sqrt{2}}\left(|a\rangle + |a_\perp\rangle\right)$.

Similarly, from complementarity, it is required that $\langle b| \hat{A} |b\rangle = 0$, which is true only if $|a_\perp\rangle$ is the eigenstate for eigenvalue -1 of the observable $\hat{A}$. Applying this argument to all $+1$ eigenstates of A, we can write these operators as

$$\hat{A} = \textstyle\sum_a |a\rangle\langle a| - |a_\perp\rangle\langle a_\perp|, \tag{3.26a}$$

$$\hat{B} = \textstyle\sum_a |a_\perp\rangle\langle a| + |a\rangle\langle a_\perp|, \tag{3.26b}$$

and the operators have the same dimensionality. It is easy to verify that these two operators anticommute,

$$\begin{aligned}\{\hat{A}, \hat{B}\} = \sum_a \Big[&(|a\rangle\langle a| - |a_\perp\rangle\langle a_\perp|)(|a_\perp\rangle\langle a| + |a\rangle\langle a_\perp|) \\ &+ (|a_\perp\rangle\langle a| + |a\rangle\langle a_\perp|)(|a\rangle\langle a| - |a_\perp\rangle\langle a_\perp|)\Big] \\ &= \sum_a [(|a\rangle\langle a_\perp| - |a_\perp\rangle\langle a|) + (|a_\perp\rangle\langle a| - |a\rangle\langle a_\perp|)] \\ &= 0.\end{aligned} \tag{3.27}$$

□

Theorem 3.3.2. *For a set of anticommuting dichotomic observables* $\{\hat{A}_j\}$ *with eigenvalues* $+1$ *and* -1*, the following inequality holds*

$$\sum_j \alpha_j^2 \leqslant 1, \tag{3.28}$$

where α_j *are the expectation value of the operators* $\hat{A}_j$*.*

Proof. Consider a set of anticommuting operators $\{\hat{A}_j\}$. Define the operator $\hat{F} \equiv \sum_j \alpha_j \hat{A}_j$, where $\alpha_j = \langle \hat{A}_j \rangle$ and $|\alpha_j| \leqslant 1$. Taking the variance of F, one obtains $\langle \hat{F}^2 \rangle - \langle \hat{F} \rangle^2 = \left(\sum_j \alpha_j^2\right)^2 - \sum_j \alpha_j^2 \geqslant 0$. Hence

$$\sum_j \alpha_j^2 \leqslant 1, \tag{3.29}$$

which completes the proof. □

With these two theorems, it is easy to see how the upper bound for the quantum mechanical bound of the Bell parameter in equation (3.17) can be obtained.

Since Pauli operators are dichotomic observables and, hence, tensor products of Pauli operators, $\hat{T}_{x_1...x_N} = \sigma^1_{x_1} \otimes ... \otimes \sigma^N_{x_N}$ are also dichotomic observables, then by Theorem (3.3.1) the operators $\hat{T}_{x_1...x_N}$ anticommute if they are complementary. Hence it is possible to group these operators into sets, S_j, where every operator in each set anticommutes with one another. S_j is known as *anticommuting set*. Writing the expectation value of the operators, $T_{x_1...x_N} = \text{tr}(\hat{T}_{x_1...x_N}.\rho)$, in each set as a vector, $\vec{S}_j$, then by Theorem (3.3.2) the squared norm of this vector is bounded by 1. Hence one can calculate the quantum bound of the Bell parameter by finding the minimum number of anticommuting sets for the operators $\hat{T}_{x_1...x_N}$ in equation (3.17),

$$\mathcal{B}^2 \leqslant \sum_{x_1,...,x_N=1}^{2} T^2_{x_1...x_N} \leqslant \text{minimum number anticommuting sets} \tag{3.30}$$

3.3.2 Alternate derivation on the bound

The entropic uncertainty relation describes the uncertainty relation for incompatible observables in information theoretic framework. In [4] the authors provided a technique to obtain the entropic uncertainty relations for dichotomic observables using their anticommutation relations. Apart from obtaining the entropic uncertainty relations, we notice that this technique is also able to obtain a stricter bound for the Bell monogamy relations than the complementarity principle, or at least reduces to Theorem (3.3.2). In this section, we will only provide relevant parts of the technique presented in the paper to show how it is stronger than the complementarity principle, and how it reduces back to Theorem (3.3.2) when we relax the condition.

Assuming that there is a set of dichotomic observables $\{\hat{A}_1, ..., \hat{A}_M\}$, the anticommutation matrix T is defined where it matrix elements are $[T]_{j,k} = \frac{\mathrm{tr}(\{\hat{A}_j, \hat{A}_k\}.\rho)}{2}$. Furthermore, define the vector α where $\alpha_j = \mathrm{tr}(A_j \rho)$ as in equation (3.28).

Consider the operator

$$\hat{K} = \sum_j a_j \hat{A}_j, \tag{3.31}$$

where $a = (a_1, ..., a_M)^{\mathrm{T}}$ is any arbitrary real unit vector, and the superscript T means taking the transpose. The trick here is to apply the Cauchy-Schwarz inequality $\left[\mathrm{tr}(X^\dagger Y)\right]^2 \leqslant \mathrm{tr}(X^\dagger X).\mathrm{tr}(Y^\dagger Y)$; setting $X = \hat{K}\sqrt{\rho}$ and $Y = \sqrt{\rho}$,

$$\begin{aligned}
\left[\mathrm{tr}(\hat{K}\rho)\right]^2 &= \left[\sum_j a_j \mathrm{tr}(\hat{A}_j \rho)\right]^2 \\
&= (a^{\mathrm{T}}\alpha)(\alpha^{\mathrm{T}} a) \\
&\leqslant \mathrm{tr}[(\hat{K}\sqrt{\rho})^\dagger (\hat{K}\sqrt{\rho})]\mathrm{tr}(\sqrt{\rho}^\dagger \sqrt{\rho}) \\
&= \mathrm{tr}(\hat{K}^2 \rho) \\
&= \sum_{j,k} a_j a_k \mathrm{tr}(A_j A_k \rho) \\
&= \sum_{j,k} a_j a_k [T]_{j,k} \\
&= a^{\mathrm{T}} T a.
\end{aligned} \tag{3.32}$$

The inequality (3.32) holds for any general real unit vector a, hence the following operator inequality holds,

$$\alpha\alpha^{\mathrm{T}} \leqslant T. \tag{3.33}$$

The inequality (3.33) reduces to Theorem (3.3.2) in complementarity principle. This can be readily seen by assuming that the set dichotomic observables are all anticommuting, $\frac{\{\hat{A}_j, \hat{A}_k\}}{2} = \delta_{jk}$. The anticommutation matrix T is, hence, the identity matrix. Letting $a = \frac{\alpha}{|\alpha|}$ where $|\alpha| = \sqrt{\alpha^{\mathrm{T}}\alpha}$, inequality (3.32) reduces to $\left(\sum_j \alpha_j^2\right)^2 \leqslant 1$ which is equivalent to equation (3.28). Inequality (3.33) is stronger than the complementarity principle because it is not limited to only anticommuting operators; it is at least as strong as equation (3.28).

3.3.3 Examples using complementarity to obtain the Bell monogamy relation

We will give two examples to illustrate how the complementarity principle can be used to obtain the bound for the Bell parameter.

The monogamy of two CHSH inequalities in equation (2.10) can be obtained from the complementarity principle. The operators involved in $\mathcal{B}^2_{AB^1}$ are $\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{210}, \hat{T}_{220}\}$, and the operators involved in $\mathcal{B}^2_{AB^2}$ are $\{\hat{T}_{101}, \hat{T}_{102}, \hat{T}_{201}, \hat{T}_{202}\}$. These operators can be rearranged into two anticommuting sets, $\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{201}, \hat{T}_{202}\}$ and $\{\hat{T}_{210}, \hat{T}_{220}, \hat{T}_{101}, \hat{T}_{102}\}$. Hence the bound from complementarity principle is $\mathcal{B}^2_{AB^1} + \mathcal{B}^2_{AB^2} \leqslant 2$. Any theory that predicts a higher value would necessarily violate the complementarity principle.

The second example we will look at is the monogamy of observer $\{1, 2\}$, $\{1, 3\}$ and $\{2, 3\}$, as in the case in Section (3.2). The operators involved in $\mathcal{B}^2_{12}$, $\mathcal{B}^2_{13}$ and $\mathcal{B}^2_{23}$ are $\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{210}, \hat{T}_{220}\}$, $\{\hat{T}_{101}, \hat{T}_{102}, \hat{T}_{201}, \hat{T}_{202}\}$ and $\{\hat{T}_{011}, \hat{T}_{012}, \hat{T}_{021}, \hat{T}_{022}\}$ respectively. These operators can be sorted into 4 anticommuting sets; the bound from complementarity principle is 4. One such arrangement is $\{\hat{T}_{110}, \hat{T}_{201}, \hat{T}_{022}\}$, $\{\hat{T}_{120}, \hat{T}_{202}, \hat{T}_{011}\}$, $\{\hat{T}_{210}, \hat{T}_{102}, \hat{T}_{021}\}$ and $\{\hat{T}_{220}, \hat{T}_{101}, \hat{T}_{012}\}$. However, as seen in equation (3.25), the bound is at most 3. So is the complementarity principle not good in obtaining the bound for this case? Apparently we can refine the techniques of complementarity to obtain the bound of 3. We call this method *duplication of operators.*

As the name suggest, we duplicate the operators involved in the Bell monogamy such that there are two copies each ($2\mathcal{B}^2_{12}$, $2\mathcal{B}^2_{13}$ and $2\mathcal{B}^2_{23}$): $\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{210}, \hat{T}_{220}\}$, $\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{210}, \hat{T}_{220}\}$, $\{\hat{T}_{101}, \hat{T}_{102}, \hat{T}_{201}, \hat{T}_{202}\}$, $\{\hat{T}_{101}, \hat{T}_{102}, \hat{T}_{201}, \hat{T}_{202}\}$, $\{\hat{T}_{011}, \hat{T}_{012}, \hat{T}_{021}, \hat{T}_{022}\}$ and $\{\hat{T}_{011}, \hat{T}_{012}, \hat{T}_{021}, \hat{T}_{022}\}$. We can arrange these operators into 6 anticommuting sets:

$$\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{201}, \hat{T}_{202}\}, \tag{3.34a}$$

$$\{\hat{T}_{110}, \hat{T}_{210}, \hat{T}_{021}, \hat{T}_{022}\}, \tag{3.34b}$$

$$\{\hat{T}_{210}, \hat{T}_{220}, \hat{T}_{101}, \hat{T}_{102}\}, \tag{3.34c}$$

$$\{\hat{T}_{120}, \hat{T}_{220}, \hat{T}_{011}, \hat{T}_{012}\}, \tag{3.34d}$$

$$\{\hat{T}_{101}, \hat{T}_{201}, \hat{T}_{012}, \hat{T}_{022}\}, \tag{3.34e}$$

$$\{\hat{T}_{102}, \hat{T}_{202}, \hat{T}_{011}, \hat{T}_{021}\}. \tag{3.34f}$$

Hence the bound from complementarity is $\mathcal{B}_{12}^2 + \mathcal{B}_{13}^2 + \mathcal{B}_{23}^2 \leqslant 6/2 = 3$.

As the duplication of operators method is often not obvious, we have devised a simplification of this method which we call the *averaging* method. We notice that this Bell monogamy relation can be obtained by averaging three bipartite relations, namely

$$\begin{aligned} \mathcal{B}_{12}^2 + \mathcal{B}_{13}^2 &\leqslant 2, \\ \mathcal{B}_{12}^2 + \mathcal{B}_{23}^2 &\leqslant 2, \\ \mathcal{B}_{13}^2 + \mathcal{B}_{23}^2 &\leqslant 2. \end{aligned} \tag{3.35}$$

The operators for the monogamy relation $\mathcal{B}_{12}^2 + \mathcal{B}_{13}^2$ are in equations (3.34a,3.34c), for $\mathcal{B}_{12}^2 + \mathcal{B}_{23}^2$ are in equations (3.34b,3.34d), and for $\mathcal{B}_{13}^2 + \mathcal{B}_{23}^2$ are in equations (3.34e,3.34f). Adding these three bipartite relations together and simplifying the inequality, we obtain the needed monogamy relation

$$\begin{aligned} \mathcal{B}_{12}^2 + \mathcal{B}_{13}^2 + \mathcal{B}_{12}^2 + \mathcal{B}_{23}^2 + \mathcal{B}_{13}^2 + \mathcal{B}_{23}^2 &\leqslant 2 + 2 + 2, \\ \mathcal{B}_{12}^2 + \mathcal{B}_{13}^2 + \mathcal{B}_{23}^2 &\leqslant 3. \end{aligned} \tag{3.36}$$

Other than obeying equation (3.36), the subsystems must also obey the relations in equation (3.35) as was mention in the last sentence of Section (3.2).

We note that the inequalities in equation (3.35) are of a certain form, $\mathcal{B}^2_{AB^1} + \mathcal{B}^2_{AB^2} \leqslant 2$. We call this the elementary bipartite Bell monogamy relations. It is called the elementary relation because it can be used to obtain any arbitrary bipartite monogamy relations by the method of *averaging*; it is the building block for any arbitrary bipartite systems. We will study more on bipartite and tripartite elementary relations in the next chapter.

3.3.4 Algorithm to solve for the bound

The bound obtained from complementarity principle is based on arranging the operators into as little anticommuting sets as possible. This can be translated into a well-known problem in graph theory, *clique cover problem*.

We construct the *anticommuting graph* and find its minimum clique cover number. The minimum clique cover number of a graph is the minimum number of cliques needed to cover all the vertices in the graph.

The vertex set of the anticommuting graph consist of the operators involved in the Bell monogamy. Two vertices are connected with an edge if they anticommute. An example of the anticommuting graph of $\mathcal{B}^2_{12} + \mathcal{B}^2_{13}$ is shown in Figure (3.4).

The minimum clique cover problem can be solved exactly by solving the chromatic number of its complement graph. A complement graph has the same vertex set as the original graph, and two vertices are adjacent if they are not in the original graph.

This is a NP-complete problem and hence the runtime increases rapidly as the number of operators increases. We have seen that to obtain a good bound from complementarity we may need to use the method of *duplication of operators* in Subsection (3.3.3), therefore the computational time needed maybe very long even for small systems. We provided an algorithm in Appendix (F) to solve the clique cover problem.

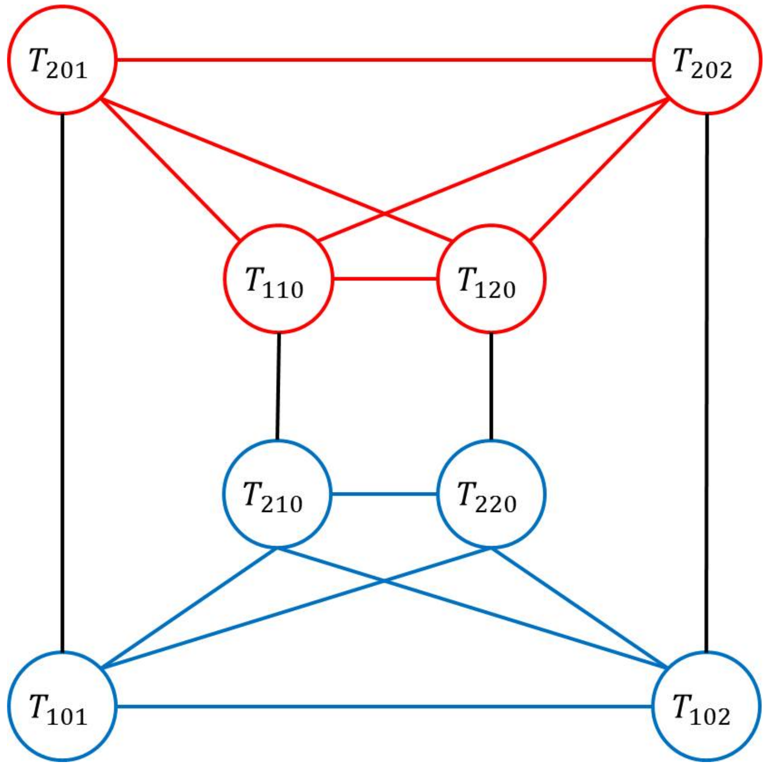


Figure 3.4: This graph shows the anticommuting graph for the monogamy of $\mathcal{B}_{12}^2$ and $\mathcal{B}_{13}^2$. Every vertex represents an operator involved in the Bell monogamy. Two vertices are connect with an edge if they anticommute. The minimum clique cover number is 2 as shown by the two cliques in red and blue.

The greedy algorithm can be used as an approximate solution to the clique cover problem. The greedy algorithm operates by listing and ranking all the cliques according to their number of vertices in each stage and choosing only the clique with the greatest number of vertices. In this thesis we are only interested in exact solutions, hence we will not use this algorithm.

We also mentioned the *averaging* method in (3.3.3). This method can be translated to the *subgraph isomorphism problem*.

Construct the hypergraph of the k-partite system as in Section (2.3). Find all subgraphs isomorphic to the elementary monogamy relations. These subgraphs represent Bell monogamy relations. After that, find the overall Bell monogamy relation by averaging these Bell monogamy relations. An example can be found in Section (4.2).

We did not provide an algorithm for the method of averaging as subgraph isomorphism problem is hard to implement, and the elementary relations are different for different number of parties. Furthermore, subgraph isomorphism problem is also NP-complete, and hence the runtime is not significantly improved compared to the duplication of operators method.

Chapter 4

Bell Monogamy Relation

Bell monogamy relation was introduced in Chapter (2.3). In this chapter, we will only look at Bell monogamy relations with quadratic Bell parameters. We will define two more concepts; *tight* Bell monogamy relations and *elementary* Bell monogamy relations.

Definition 4.0.1. The monogamy relation is called *tight* if there exist a quantum state that saturates the bound of the Bell monogamy relation.

Definition 4.0.2. A monogamy relation is called *elementary* if it cannot be obtained by averaging from other elementary monogamy relations.

Elementary relations are like prime numbers. Any monogamy relations that cannot be obtained from the elementary monogamy relations are, themselves, elementary relations.

4.1 Bipartite monogamy relation

There is only one elementary monogamy relation for bipartite monogamy. The elementary monogamy relation is

$$\mathcal{B}_{12}^2 + \mathcal{B}_{13}^2 \leqslant 2. \tag{4.1}$$

We can use this monogamy relation to obtain the monogamy relations for any arbitrary bipartite graph. The method presented below is based on the method of averaging.

1. Construct the bipartite graph G for any arbitrary system where each vertex represents an observer and two vertices are adjacent if the corresponding observers are involved in a Bell parameter. Each edge of G represents the Bell parameter of its vertices.

2. Construct the line graph $L(G)$. The vertices of the line graph $v \in V(L)$ are the edges of G. The vertices of $L(G)$ are adjacent if the corresponding edges are incident in G. Hence the vertex set $V(L)$ is the set of Bell parameters, and the edge set $E(L)$ is the set of monogamy relations. The $E(L)$ is equivalent to identifying all the isomorphic elementary Bell monogamy subgraphs from G.

3. The elementary Bell monogamy relations identified in $E(L)$ are summed up by

$$\sum_v d_v \mathcal{B}_v^2 \leqslant 2\epsilon, \tag{4.2}$$

   where d_v are the degree of the vertices v, and $\epsilon = |E(L)|$ is the cardinality of the edge set of L.

Equation (4.2) is tight. Since $\sum_v d_v = 2\epsilon$ from the handshaking lemma, the bound can be saturated by assuming that all $B_v = 1$ which is achievable because it is within

LHV bound in equation (3.17). Hence this equation is the general monogamy relation for any bipartite relations. An example of a bipartite line graph is shown in Figure (4.1).

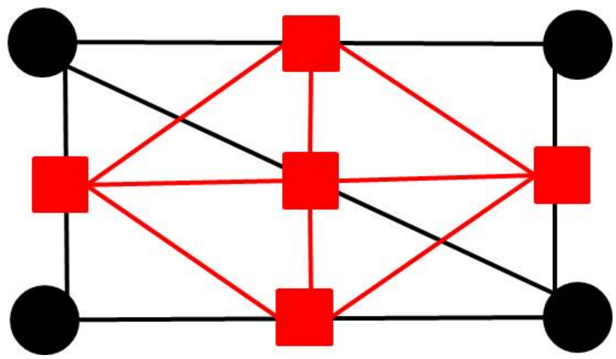


Figure 4.1: The black dots and black lines are vertices and edges of an arbitrary bipartite graph G. The red squares and red lines are vertices and edges of its line graph $L(G)$. The red dots represent the Bell parameter and the red lines represent a monogamy relation.

4.2 Tripartite monogamy relation

We are able to obtain tight bipartite monogamy relation for any arbitrary bipartite graphs from the elementary bipartite monogamy relation. It is natural to generalise this idea to multipartite case. However, the extension to multipartite case is not trivial. The simplest case to study is, probably, the tripartite case, and for the rest of the thesis we will look at tripartite monogamy relations.

4.2.1 Elementary tripartite monogamy relations

As in the bipartite case, we try to identify the elementary tripartite monogamy relations. We have found three elementary relations so far using the complementarity principle:

$$\text{Square graph: } \mathcal{B}_{123}^2 + \mathcal{B}_{234}^2 + \mathcal{B}_{341}^2 + \mathcal{B}_{412}^2 \leqslant 4, \tag{4.3a}$$

$$\text{Pyramid graph: } \mathcal{B}_{123}^2 + \mathcal{B}_{345}^2 + \mathcal{B}_{561}^2 + \mathcal{B}_{135}^2 \leqslant 4, \tag{4.3b}$$

$$\text{Frankenstein graph: } \mathcal{B}_{123}^2 + \mathcal{B}_{124}^2 + \mathcal{B}_{156}^2 + \mathcal{B}_{157}^2 \leqslant 4. \tag{4.3c}$$

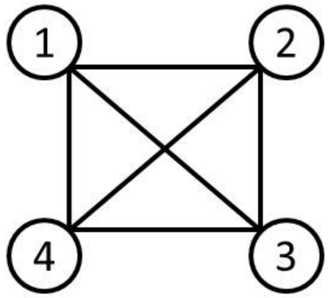
The names of the elementary relations are of various reasons. The square graph is the first elementary relation found and its tripartite graph looks like a square. The pyramid graph is the second elementary graph found and the KF representation looks like a pyramid. KF representation is an alternate representation that we will introduce later on. The frankenstein graph is the most recent discovery and it was constructed from the bipartite elementary relation, and hence its name. We will show how to construct the frankenstein graph later on too.

Another way to represent the tripartite graph is the KF representation (the name is tentative). This representation is just neater than the original tripartite graph. To convert a tripartite graph to the KF graph, represent each hyperedge in the tripartite graph as a triangle and the vertices in the hyperedge as the vertices on the triangle. The KF graph for the three elementary tripartite monogamy relations are shown in Figure (4.2).

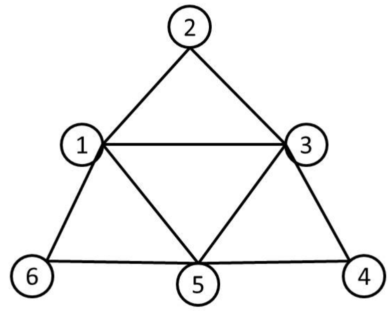
The pitfall using this representation is that it may erroneously represent Bell parameters that are not in the monogamy relation. For example, the KF graph for $\mathcal{B}_{123}^2 + \mathcal{B}_{345}^2 + \mathcal{B}_{561}^2$ is the same as the pyramid graph in Figure (4.2b), but the pyramid graph suggests an additional term $\mathcal{B}_{135}^2$.

4.2.2 Examples on interesting tripartite monogamy relations

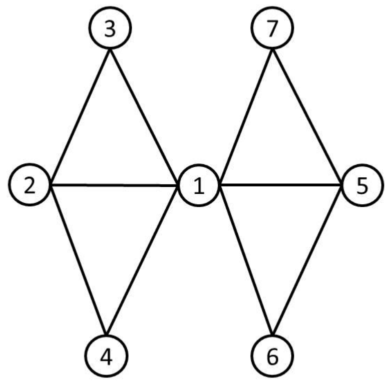
We can derive many monogamy relations from the elementary monogamy relations in equation (4.3). We will see some of the interesting examples in this subsection.



(a) Square graph.



(b) Pyramid graph.



(c) Frankenstein graph.

Figure 4.2: KF representations of the three elementary tripartite monogamy relations.

We can obtain simpler monogamy relations from the elementary relations. For example, we can obtain the bound $\mathcal{B}_{123}^2 + \mathcal{B}_{234}^2 \leqslant 4$ by setting $\mathcal{B}_{341}^2 + \mathcal{B}_{412}^2 = 0$ in equation (4.3a), and $\mathcal{B}_{123}^2 + \mathcal{B}_{345}^2 \leqslant 4$ by setting $\mathcal{B}_{561}^2 + \mathcal{B}_{135}^2 = 0$ in equation (4.3b). We can obtain other simpler monogamy relations by setting different Bell parameters to zero in the elementary tripartite monogamy relations.

Similarly, we can obtain composite monogamy relations by mixing different monogamy relations. For example, we can obtain the bound $\mathcal{B}_{123}^2 + \mathcal{B}_{345}^2 + \mathcal{B}_{561}^2 + \mathcal{B}_{135}^2 + \mathcal{B}_{726}^2 + \mathcal{B}_{246}^2 + \mathcal{B}_{647}^2 + \mathcal{B}_{472}^2 \leqslant 8$ by combining equation (4.3b) and (4.3a). The first four Bell parameters form the pyramid graph and the last four Bell parameters form the square graph. The KF graph of this example is in Figure (4.3).

We can use the method of averaging to obtain monogamy relations as well. For example, we can obtain the bound on $\mathcal{B}_{123}^2 + \mathcal{B}_{234}^2 + \mathcal{B}_{341}^2 + \mathcal{B}_{412}^2 + \mathcal{B}_{125}^2 \leqslant 6$ (house graph)

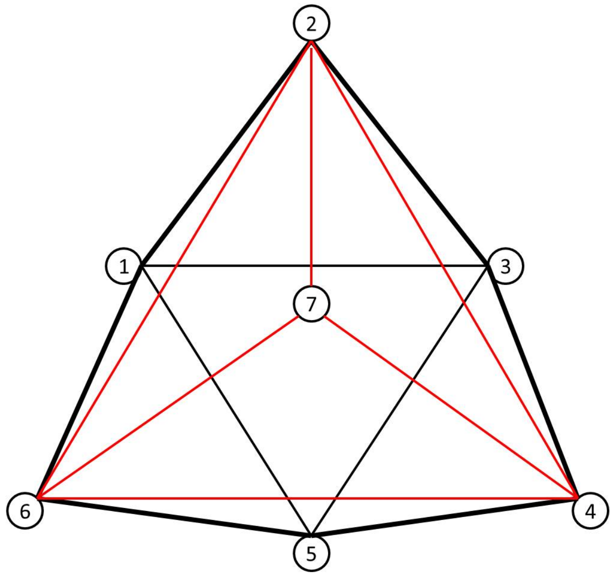


Figure 4.3: The KF graph of the composite of the pyramid graph with the square graph. The pyramid graph is seen by the black lines and the square graph is seen by the red lines.

by identifying the subgraphs isomorphic to the elementary monogamy relations (or their subgraphs). The equations in (4.4) are the isomorphic subgraphs. A KF graph for the house graph is shown in Figure (4.4).

$$\begin{aligned}
&\text{From square: } \mathcal{B}_{123}^2 + \mathcal{B}_{234}^2 + \mathcal{B}_{341}^2 + \mathcal{B}_{412}^2 \leqslant 4 \\
&\text{From pyramid: } \mathcal{B}_{125}^2 + \mathcal{B}_{124}^2 + \mathcal{B}_{134}^2 \leqslant 4 \\
&\text{From pyramid: } \mathcal{B}_{125}^2 + \mathcal{B}_{124}^2 + \mathcal{B}_{234}^2 \leqslant 4 \\
&\text{From pyramid: } \mathcal{B}_{125}^2 + \mathcal{B}_{123}^2 + \mathcal{B}_{134}^2 \leqslant 4 \\
&\text{From pyramid: } \mathcal{B}_{125}^2 + \mathcal{B}_{123}^2 + \mathcal{B}_{234}^2 \leqslant 4
\end{aligned} \tag{4.4}$$

As seen in the example for house graph, the averaging method involves searching for subgraphs isomorphic to the elementary graphs. This method is NP-complete and is also hard to implement.

The final example we will look at is the full tripartite graph. A full tripartite graph with N observers, denoted by $\mathsf{K}_{3,N}$, involves all possible combinations of Bell

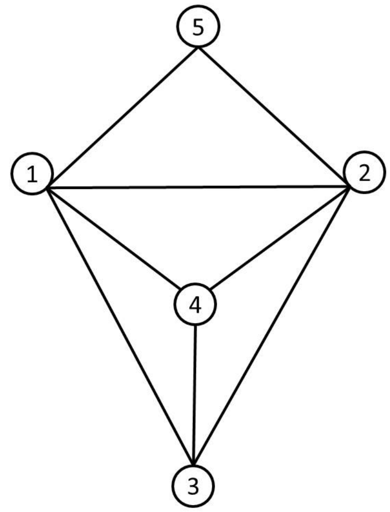


Figure 4.4: The KF graph the house graph. Its original tripartite graph looks like a house, hence its name. There are many isomorphic elementary subgraphs in this house graph.

parameters. Since it is a full graph, there are $\binom{N}{3}$ Bell parameters in the monogamy relation.

Theorem 4.2.1. *The Bell monogamy relation of a full tripartite graph, $\mathsf{K}_{3,N}$ where $N \geqslant 4$ is*

$$\sum_{j=1}^{\binom{N}{3}} \mathcal{B}_j^2 \leqslant \binom{N}{3}, \tag{4.5}$$

and is tight.

Proof. We will prove Theorem (4.2.1) by induction.

For $N = 4$, we see that the full graph is the square graph, and hence equation (4.5) is satisfied.

Assume that $N = k$ is true for $k > 4$ such that

$$\sum_{j=1}^{\binom{k}{3}} \mathcal{B}_j^2 \leqslant \binom{k}{3}. \tag{4.6}$$

A full graph, $\mathsf{K}_{3,k+1}$ has $(k+1)$ subgraphs of $\mathsf{K}_{3,k}$. As each Bell parameter appears $(k-2)$ times when summing up all the $(k+1)$ subgraphs, the full graph Bell monogamy relation for $\mathsf{K}_{3,k+1}$ is

$$\sum_{j=1}^{\binom{k+1}{3}} \mathcal{B}_j^2 \leqslant \frac{(k+1)\binom{k}{3}}{k-2} = \binom{k+1}{3}, \tag{4.7}$$

thereby showing that the monogamy relation holds for $N = k + 1$.

Since the basis and the inductive step are true, by mathematical induction, Theorem (4.2.1) holds for $N \geqslant 4$.

We can easily see that the monogamy relation for the tripartite full graph is tight as we can saturate the bound by having $\mathcal{B}_j = 1$. □

4.2.3 Frankenstein graph

Frankenstein graph in equation (4.3c) is a constructed elementary monogamy relation that was discovered by sewing two bipartite monogamy relations together. We will show how this was done and how this technique can be used to obtain elementary monogamy relations for higher partite graphs.

We start off by writing the operators for the elementary bipartite Bell monogamy relation in two anticommuting sets as in equation (4.8),

$$\begin{aligned} &\{\hat{T}_{110}, \hat{T}_{120}, \hat{T}_{201}, \hat{T}_{202}\}, \\ &\{\hat{T}_{210}, \hat{T}_{220}, \hat{T}_{101}, \hat{T}_{102}\}. \end{aligned} \tag{4.8}$$

We tensor product $\hat{T}_{000}$ and $\{\sigma_1, \sigma_2\}$ on the left of all the operators in equation (4.8). Now we have four sets of anticommuting operators as shown in equation (4.9).

$$\{\hat{T}_{0001110}, \hat{T}_{0001120}, \hat{T}_{0001201}, \hat{T}_{0001202}\}, \tag{4.9a}$$

$$\{\hat{T}_{0001210}, \hat{T}_{0001220}, \hat{T}_{0001101}, \hat{T}_{0001102}\}, \tag{4.9b}$$

$$\{\hat{T}_{0002110}, \hat{T}_{0002120}, \hat{T}_{0002201}, \hat{T}_{0002202}\}, \tag{4.9c}$$

$$\{\hat{T}_{0002210}, \hat{T}_{0002220}, \hat{T}_{0002101}, \hat{T}_{0002102}\}. \tag{4.9d}$$

Now, copying and reflecting the four qubit system in equation (4.9) about the forth qubit, we obtain

$$\{\hat{T}_{0111000}, \hat{T}_{0211000}, \hat{T}_{1021000}, \hat{T}_{2021000}\}, \tag{4.10a}$$

$$\{\hat{T}_{0121000}, \hat{T}_{0221000}, \hat{T}_{1011000}, \hat{T}_{2011000}\}, \tag{4.10b}$$

$$\{\hat{T}_{0112000}, \hat{T}_{0212000}, \hat{T}_{1022000}, \hat{T}_{2022000}\}, \tag{4.10c}$$

$$\{\hat{T}_{0122000}, \hat{T}_{0222000}, \hat{T}_{1012000}, \hat{T}_{2012000}\}. \tag{4.10d}$$

These eight operators in equation (4.9) and (4.10) can be group into four anticommuting sets by taking the union of set (4.9a) and (4.10c), set (4.9b) and (4.10d), set (4.9c) and (4.10a), and set (4.9d) and (4.10b). This is exactly the operators in frankenstein graph.

This method can be used to obtain "frankenstein" elementary monogamy relations of higher partite systems. We will summarize the steps to obtain the frankensteins for k-partite system below.

1. Choose any two elementary Bell monogamy relations, $\mathcal{E}_1$ and $\mathcal{E}_2$, from $(k-1)$-partite system. The number of qubits involved in the monogamy relations are n_1 and n_2 respectively.

2. Group the operators of $\mathcal{E}_1$ and $\mathcal{E}_2$ into anticommuting sets. The set of anticommuting sets are denoted by $\mathcal{S}_1$ and $\mathcal{S}_2$ respectively, and the number of anticommuting sets in each set is denoted by $|\mathcal{S}_j|$

3. Tensor product $\hat{T}_2 = \sigma_0^{\otimes n_2}$ with $\{\sigma_1, \sigma_2\}$ on the left of $\mathcal{E}_1$ and $\{\sigma_1, \sigma_2\}$ with $\hat{T}_1 = \sigma_0^{\otimes n_1}$ the right of $\mathcal{E}_2$. Hence the number of anticommuting sets in $\mathcal{E}_1$ and $\mathcal{E}_2$ are doubled, i.e. $|\mathcal{S}_1'| = 2|\mathcal{S}_1|$ and $|\mathcal{S}_2'| = 2|\mathcal{S}_2|$.

4. It is now possible to merge $\mathcal{S}_1'$ and $\mathcal{S}_2'$ to form $\mathcal{S}$ such that $|\mathcal{S}| = |\mathcal{S}_j'|$ like how we merge set (4.9) and (4.10). We have now constructed the k-partite frankenstein Bell monogamy relation $\mathcal{E}$ corresponding to $\mathcal{S}$.

4.2.4 Problems in elementary Bell monogamy relations

Despite the fact that we can use the three elementary tripartite monogamy relations to obtain other more complicated monogamy relations, these monogamy relations may not be tight. We will look at a class of monogamy relation, the cycle graph, in this subsection and discuss on its tightness.

Definition 4.2.1. An M-cycle tripartite graph consists of M hyperedges and $2M$ vertices. The hyperedges can be placed around a circle and two hyperedges share a common vertex if they are beside each other. The Bell monogamy relation for an M-cycle graph is of the form $\mathcal{B}_{123}^2 + \mathcal{B}_{345}^2 + \mathcal{B}_{567}^2 + ... + \mathcal{B}_{(2M-1)(2M)1}^2$.

A M-cycle tripartite graph has the monogamy relation

$$\sum_{j=1}^{M} \mathcal{B}_j^2 \leqslant 2M. \tag{4.11}$$

The bound is saturated for even cycles. The state with alternating GHZ states and eigenstates of the σ_1 will do the job,

$$\begin{aligned}|\psi\rangle = |GHZ\rangle_{123} \otimes \frac{|0\rangle_4 \pm |1\rangle_4}{\sqrt{2}} \otimes |GHZ\rangle_{567} \otimes \frac{|0\rangle_8 \pm |1\rangle_8}{\sqrt{2}} \otimes \\ ... \otimes |GHZ\rangle_{(2M-3)(2M-2)(2M-1)} \otimes \frac{|0\rangle_{2M} \pm |1\rangle_{2M}}{\sqrt{2}}.\end{aligned} \tag{4.12}$$

No conclusion on the tightness of the monogamy relations for odd cycles with $M > 3$ can be made so far; we have found no state that saturates the bound, nor do we have a proof that the bound is not tight. We conjecture that such a state does not exist and hence the bound is not tight. As such, if our conjecture is true, all odd cycle tripartite monogamy relations must be added to the set of elementary monogamy relations.

We have clues on the properties of the quantum state if it saturates the bound.

Property 1. There exist a pure state that saturates the bound.

Property 2. All the square of the Bell parameters must equal to 2, i.e. $\mathcal{B}_j^2 = 2$.

Property 3. There exist a pure state for the subsystem $\{\mathcal{B}_{123}, \mathcal{B}_{345}, \mathcal{B}_{567}\}$ such that the square of each Bell parameter equals 2.

We will look at the 5-cycle graph as an example to prove the three properties. Generalising it to M-cycle is a simple extension.

Property 1. can be proven as follows. Consider a general state $\rho = \sum_k p_k \left|\phi\right\rangle_k \left\langle\phi\right|_k$. The monogamy relation is calculated as

$$\begin{aligned}
\mathcal{B}^2 &= 10 && (4.13a)\\
&= \sum_j \left[\mathrm{tr}(\hat{T}_j \rho)\right]^2 && (4.13b)\\
&= \sum_j \left[\mathrm{tr}(\hat{T}_j \sum_k p_k \left|\phi\right\rangle_k \left\langle\phi\right|_k)\right]^2 && (4.13c)\\
&= \sum_j \left[\sum_k p_k T_j(\phi_k)\right]^2 && (4.13d)\\
&\leqslant \sum_j \sum_k p_k T_j^2(\phi_k) && (4.13e)\\
&\leqslant 10. && (4.13f)
\end{aligned}$$

The step from (4.13d) to (4.13e) is due to CauchySchwarz inequality where we let $\vec{u}_1 = (\sqrt{p_1}T_j(\phi_1), ..., \sqrt{p_k}T_j(\phi_k), ...)$ and $\vec{u}_2 = (\sqrt{p_1}, ..., \sqrt{p_k}, ...)$ and $(\vec{u}_1.\vec{u}_2)^2 = [\sum_k p_k T_j(\phi_k)]^2 \leqslant |\vec{u}_1|^2 |\vec{u}_2|^2 = \sum_k p_k T_j^2(\phi_k)$. The equation (4.13) is equality if and only if $\sum_j T_j^2(\phi_k) = 10$, and this completes the proof.

Property 2. can be easily seen when we write down all the isomorphic monogamy relations of the 5-cycle graph,

$$\begin{aligned}
\mathcal{B}_{123}^2 + \mathcal{B}_{345}^2 &= 4, && (4.14a)\\
\mathcal{B}_{345}^2 + \mathcal{B}_{567}^2 &= 4, && (4.14b)\\
\mathcal{B}_{567}^2 + \mathcal{B}_{789}^2 &= 4, && (4.14c)\\
\mathcal{B}_{789}^2 + \mathcal{B}_{9\,10\,1}^2 &= 4, && (4.14d)\\
\mathcal{B}_{9\,10\,1}^2 + \mathcal{B}_{123}^2 &= 4. && (4.14e)
\end{aligned}$$

If $\mathcal{B}_{123}^2 > 2$, then $\mathcal{B}_{345}^2 < 2$, $\mathcal{B}_{567}^2 > 2$, $\mathcal{B}_{789}^2 < 2$, $\mathcal{B}_{9\,10\,1}^2 > 2$, and finally $\mathcal{B}_{123} < 2$ which leads to a contradiction. Hence all Bell parameters must be equal to 2.

Property 3. is a corollary of Property 1. and Property 2.. We start with a pure state that saturates the bound and trace out qubit 8, 9 and 10. The reduce density matrix of the subsystem must saturate the bound for the monogamy $\mathcal{B}_{123}^2 + 2\mathcal{B}_{345}^2 + \mathcal{B}_{567}^2 = 8$. The proof for Property 1. can hence be used to show that there exist a pure state that saturates the bound for the monogamy of the subsystem.

After all the effort, we have reduced the problem to finding a pure state that satisfy Property 3.. If Property 3. is shown to be not true, and no such state exist, then it implies that all odd cycle graphs cannot be obtained from elementary monogamy relations (at least from complementarity principle alone) and must be added to the elementary set.

Chapter 5

Conclusion

In this project, we have explored some principles and methods to obtain Bell monogamy relations.

From the no-signalling principle, we formulated a new method within graph theory to obtain any arbitrary multipartite monogamy relations. This is in contrast with the method used in the paper [21] where it is only suitable for bipartite monogamy relations.

We provided an alternative proof for the method to obtain the Bell monogamy relation from complementarity principle. This alternative proof also contains a stronger relation than the one in complementarity principle.

Using the complementarity principle, it was shown that arranging the operators into anticommuting sets is equivalent to the *clique cover problem*. We have provided a simple algorithm to solve this problem.

We also show two methods that refine the bound, *duplication of operators* and *averaging* method. These two methods are shown to be equivalent, and the averaging method is equivalent to the *subgraph isomorphism problem*.

Three elementary tripartite monogamy relations are also discovered, one of which is the frankenstein graph. The method for building a frankenstein graph is provided for higher partite case.

Lastly, we conjecture that all odd cycle tripartite graphs must be added into the elementary set. We also show a possible simplification of the problem that may prove the conjecture.

Appendix A

EPR Paradox

Albert Einstein, Boris Podolsky and Nathan Rosen (EPR) published their paper in 1935 to show that quantum mechanics is an incomplete theory[1].

A complete theory, according to the EPR paper, is such that "every element of physical reality must have a counterpart in the physical theory." A physical reality is defined to be "if, without in any way disturbing a system, we can predict with certainty (i.e. with probability equal to unity) the value of a physical quantity, then there exists an element of physical reality corresponding to this physical quantity." There are two more assumptions that are not explicitly stated in the EPR paper, as suggested by David Bohm [24]. The assumptions are "the world can correctly be analysed in terms of distinct and separately existing elements of reality" and "every one of these elements must be a counterpart of a precisely defined mathematical quantity appearing in a complete theory." Underlying these definitions is the concept of local realism. Realism is the idea that measurement outcomes of the elements of reality are predetermined, and locality is the idea that elements of reality cannot influence each other if they are spacelike separated.

Due to the existence of entangled states and non-commuting observables, quantum mechanics was deemed incomplete according to EPR definitions. It was demonstrated in the paper by considering the measurement of the position and momentum of a pair of entangled particles. In this thesis, we will present the version given by David Bohm[24] which considered the spin of a pair of entangled particles.

Bohm looked at a molecule containing two half-spin atoms in a state which total spin is zero; the spin of each atom is pointing in the opposite direction to each other. By some mechanism the molecule disintegrates into the two constituent atoms and they move away in opposite direction until there are no more interactions between them. As the total spin-angular momentum is conserved, the spin of the atoms are correlated.

Suppose that the spin of one the atom is measured in a certain direction, immediately the spin of the other atom in the same direction is determined unambiguously. This can be represented by the singlet state:

$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right), \tag{A.1}$$

where $\{|\uparrow\rangle, |\downarrow\rangle\}$ are eigenstates of arbitrary spin direction. Such correlation implies that either the two atoms have their spins encoded in some hidden variable and the spin of the atoms in every direction is a physical reality, or there is some instantaneous interaction between the two atoms such that their spins are always opposite when measured which violated locality.

However, in quantum mechanics, there is a basic uncertainty relation between different spin directions and it is impossible to measure to any arbitrary precision two different non-commuting spin directions. Therefore, there is no physical reality when measuring non-commuting observables and we reach a paradox. Either locality or reality is violated (or both). Hence EPR concluded that quantum mechanics is incomplete.

For example, let us assume that only one atom, atom A, is measured and the other atom, atom B, is left untouched. We will measure atom A in the z and x-direction, represented by the Pauli matrices σ_z and σ_x and the eigenstates $\{|0\rangle, |1\rangle\}$ and $\{|+\rangle, |-\rangle\}$ respectively. From Equation (A.1) when the spin of atom A in the z-direction is measured to be $|s_z\rangle_A = |0\rangle$, then the state of atom B immediately collapses to $|s_z\rangle_B = |1\rangle$, vice versa. Without disturbing atom B we determined its spin in the z-direction, hence there corresponds an element physical reality of the spin in the z-direction for atom B. Instead, if we measured the spin of atom A in the x-direction and found it to be $|s_x\rangle_A = |+\rangle$, immediately the state of atom B collapses to $|s_x\rangle_B = |-\rangle$, vice versa. Again, without disturbing atom B we determined its spin in the x-direction, hence there corresponds an element physical reality of the spin in the x-direction for atom B. However, quantum mechanics forbid us from knowing the spin of z and x-direction (incompatible observables) of atom B to any arbitrary precision due to the uncertainty principle. This is the paradox.

To sum up the paradox, the EPR argument shows that quantum mechanics does not obey local realism. The absence of local realism was paradoxical as all classical theories, including relativity, have it as their core principle. This made quantum mechanics seems incomplete.

Appendix B

Quantum Contextuality

Quantum measurements depend on the context of the measuring apparatus. One would reach a logical contradiction if one insists on having predetermined measurement results. This dependence is called quantum contextuality. This fundamental principle can also be used to obtain monogamy relations by constructing the *exclusivity graphs* and calculate its Lovász number[25]. Refer to [25] for more information on the exclusivity graph and the graph theoretic approach to finding the bound on the Bell parameter. In this chapter we will present an elegant proof of quantum contextuality as in [26].

Consider five non-contextual boxes as in Figure (B.1). There are certain conditions of finding a ball in the box for each pair of boxes. Given these conditions, one may logically deduce the joint probability distribution of finding a ball for unrelated boxes. This is the main feature of non-contextual boxes; there exists a joint probability distribution of finding a ball for all the boxes.

Study the conditions below:

1. When box 2 has a ball then box 1 is empty, and when box 2 is empty then box 3 has a ball.

2. When box 4 has a ball then box 3 is empty, and when box 4 is empty then box 5 has a ball.

These conditions can be translated to probabilities as in equation (B.1).

$$p(0,1|1,2) + p(0,1|2,3) = 1, \tag{B.1a}$$

$$p(0,1|3,4) + p(0,1|4,5) = 1, \tag{B.1b}$$

$$p(1,1|1,2) = p(0,0|2,3) = p(1,1,|3,4) = p(0,0|4,5) = 0, \tag{B.1c}$$

where $p(a, b|A, B)$ is the probability of box A being in state a and box B being in state b, and $a, b = \{0, 1\}$ where 0 means empty and 1 means has a ball.

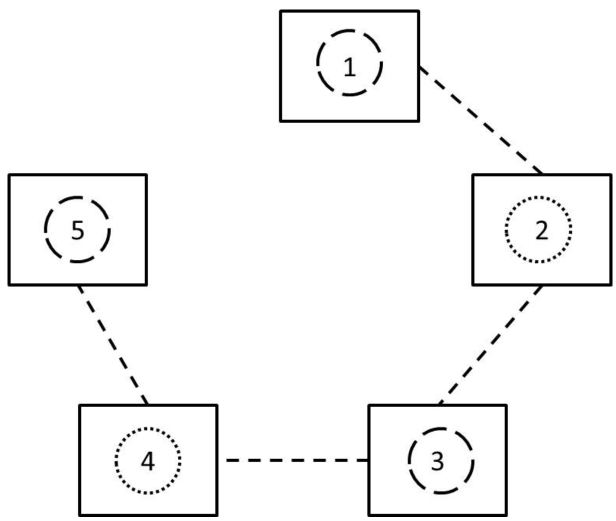


Figure B.1: The figure shows five noncontextual boxes. The dotted lines represent that either one of the two connected boxes has a ball, as in condition (B.1). This would imply that box 1, 3 and 5 all either have balls or are empty. Box 2 and 4 are related by the same manner.

With all these conditions, within non-contextual and local theories, it is obvious that $p(0, 1|5, 1) = 0$. However, it is possible to construct a quantum state and a set of quantum measurements such that the quantum state obeys condition (B.1) but $p(0, 1|5, 1) \neq 0$.

Consider the state

$$|\eta\rangle = \frac{1}{\sqrt{3}}(1, 1, 1). \tag{B.2}$$

Also consider the measurements as measuring the projector on the state $|v_j\rangle$ given by

$$|v_1\rangle = \frac{1}{\sqrt{3}}(1, -1, 1), \tag{B.3a}$$

$$|v_2\rangle = \frac{1}{\sqrt{2}}(1, 1, 0), \tag{B.3b}$$

$$|v_3\rangle = (0, 0, 1), \tag{B.3c}$$

$$|v_4\rangle = (1, 0, 0), \tag{B.3d}$$

$$|v_5\rangle = \frac{1}{\sqrt{2}}(0, 1, 1). \tag{B.3e}$$

Note that these boxes are compatible with its neighbours as shown by the orthogonal projectors. This condition is needed so that the joint probability $p(a, b|A, B)$ exists.

With simple calculations, it can be shown that conditions in (B.1) hold while $p(0, 1|5, 1) = \frac{1}{9} \neq 0$. This shows that quantum measurements depend on the context of the measuring apparatus.

Appendix C

Bell-CHSH inequality and its bounds

The correlation function is define to be

$$E(A, B) \equiv \sum_{a,b} ab\, p(a, b|A, B) = \langle ab \rangle \,, \tag{C.1}$$

where A and B are the measurement settings, a and b are the measurement outcomes, and $p(a, b|A, B)$ is the conditional joint probability of Alice and Bob obtaining outcomes a and b given that the settings are A and B respectively. $\langle ... \rangle$ denotes the expectation value of the quantity inside, hence having the same definition as the term in the middle.

Assume that there is some local hidden mechanism that determines the spin of the atom. Hence the measurement outcomes can be written as

$$a = a(A, \lambda), \tag{C.2}$$

$$b = b(B, \lambda), \tag{C.3}$$

where λ is the local hidden variable used to quantify the local hidden mechanism. Here, λ can be a variable or a set, it does not matter. Since the outcome of Alice is independent of Bob's setting and vice versa(assumption of free will and locality), we can write the conditional joint probability in equation (C.1) as[27]

$$p(a, b|A, B) = \sum_{\lambda} p(a|A, \lambda)p(b|B, \lambda)p(\lambda), \tag{C.4}$$

where $p(\lambda)$ is the probability of the atoms to be in the state λ and $\sum_{\lambda} p(\lambda) = 1$.

Combining equation (C.4) with equation (C.1), the correlation function becomes

$$E(A, B) = \sum_{\lambda} p(\lambda)\bar{a}(A, \lambda)\bar{b}(B, \lambda), \tag{C.5}$$

where $\bar{a} = \sum_a a\, p(a|A, \lambda)$ and $\bar{b} = \sum_b b\, p(b|B, \lambda)$. Since the possible values of a and b are ± 1, then

$$|\bar{a}|, |\bar{b}| \leqslant 1. \tag{C.6}$$

Consider the following equation,

$$\begin{aligned} E(A_1, B_1) - E(A_1, B_2) &= \sum_{\lambda} p(\lambda)[\bar{a}_1\bar{b}_1 - \bar{a}_1\bar{b}_2] \\ &= \sum_{\lambda} p(\lambda)\bar{a}_1\bar{b}_1[1 \pm \bar{a}_2\bar{b}_2] - \sum_{\lambda} p(\lambda)\bar{a}_1\bar{b}_2[1 \pm \bar{a}_2\bar{b}_1]. \end{aligned} \tag{C.7}$$

Applying the triangle inequality to equation (C.7), and together with equation (C.6) and the fact that $\sum_{\lambda} p(\lambda) = 1$,

$$\begin{aligned} |E(A_1, B_1) - E(A_1, B_2)| &\leqslant \left|\sum_{\lambda} p(\lambda)\bar{a}_1\bar{b}_1[1 \pm \bar{a}_2\bar{b}_2]\right| + \left|\sum_{\lambda} p(\lambda)\bar{a}_1\bar{b}_2[1 \pm \bar{a}_2\bar{b}_1]\right| \\ &\leqslant \sum_{\lambda} p(\lambda)[1 \pm \bar{a}_2\bar{b}_2] + \sum_{\lambda} p(\lambda)[1 \pm \bar{a}_2\bar{b}_1] \\ &= 2 \pm [E(A_2, B_1) + E(A_2, B_2)], \end{aligned} \tag{C.8}$$

which contains the original CHSH inequality.

Quantum mechanics allows us to violate equation (C.8). Let us consider the following scheme,

$$
\begin{aligned}
|\psi\rangle &= \frac{1}{\sqrt{2}}(|01\rangle - |10\rangle), \\
a_1 &= \sigma_z \otimes I, \\
a_2 &= \sigma_x \otimes I, \\
b_1 &= -I \otimes \frac{\sigma_z + \sigma_x}{\sqrt{2}}, \\
b_2 &= I \otimes \frac{\sigma_z - \sigma_x}{\sqrt{2}}.
\end{aligned}
$$

Calculating equation (C.8),

$$
\begin{aligned}
E(A_1, B_1) - E(A_1, B_2) + E(A_2, B_1) + E(A_2, B_2) &= \langle a_1 b_1 \rangle - \langle a_1 b_2 \rangle + \langle a_2 b_1 \rangle + \langle a_2 b_2 \rangle \\
&= 2\sqrt{2}.
\end{aligned}
\tag{C.9}
$$

Hence quantum mechanics violates the local realistic bound up to $2\sqrt{2}$.

A PR box is a no-signalling black box that exhibits more nonlocal correlations than quantum mechanics[16]. The rest of this chapter is dedicated to showing how PR box works.

For simplicity, we will relabel the measurement setting to run from 0 to 1 (only in this part). The correlations from PR box obey $\frac{|a+b|}{2} = AB$. We list down the correlations for all the settings in Table (C.1).

Table C.1: The correlations for all possible measurement settings. We can clearly see that the correlations obey no-signalling condition.

A	B	a	b
0	0	-1 1	1 -1
1	0	-1 1	1 -1
0	1	-1 1	1 -1
1	1	-1 1	-1 1

Hence it is possible to calculate the terms in the Bell-CHSH inequality:

$$E(A_1, B_1) = -1,$$

$$E(A_2, B_1) = -1,$$

$$E(A_1, B_2) = -1,$$

$$E(A_2, B_2) = 1.$$

Hence the Bell-CHSH parameter for the PR box is

$$|E(A_1, B_1) + E(A_2, B_1) + E(A_1, B_2) - E(A_2, B_2)| = 4, \tag{C.10}$$

which violates the Tsirelson bound. The PR box hence shows more nonlocal correlations that quantum mechanics but still obeying the no-signalling principle.

Appendix D

Fine's Theorem

A. Fine published an important result in his paper [14]. This result shows that an LHV model must admit a joint probability distribution for all possible measurements, and vice versa.

Theorem D.1. An LHV model exist if and only if there exist a joint probability distribution for the outcomes of all possible measurement settings.

This joint probability must return the correct marginals for all possible physical set-ups,

$$p(a_j, b_k|A_j, B_k) = \sum_{a_x|x\neq j, b_y|y\neq k} p(a_1, a_2, b_1, b_2). \tag{D.1}$$

Proof. If a system have a LHV model, then it must necessarily have

$$a = a(A, \lambda), \tag{D.2a}$$

$$b = b(B, \lambda), \tag{D.2b}$$

and

$$p(a, b|A, B) = \sum_{\lambda} p(\lambda) p(a|A, \lambda) p(b|B, \lambda). \tag{D.3}$$

A joint probability distribution can be constructed as in equation (D.4),

$$p(a_1, a_2, b_1, b_2) = \sum_{\lambda} p(\lambda)p(a_1|A_1, \lambda)p(a_2|A_2, \lambda)p(b_1|B_1, \lambda)p(b_2|B_2, \lambda), \tag{D.4}$$

where it returns all the needed marginal probabilities

$$\begin{aligned} p(a_j, b_k|A_j, B_k) &= \sum_{a_x|x\neq j, b_y|y\neq k} \sum_{\lambda} p(\lambda)p(a_1|A_1, \lambda)p(a_2|A_2, \lambda)p(b_1|B_1, \lambda)p(b_2|B_2, \lambda) \\ &= \sum_{\lambda} p(\lambda)p(a_j|A_j, \lambda)p(b_k|B_k, \lambda). \end{aligned}$$

This completes the first part of the proof.

If a system has a joint probability for all its measurements, then it is possible to construct a LHV model for it.

Define the hidden variable to be the set of all possible measurement outcomes, $\lambda = (a_1, a_2, b_1, b_2)$. Then define the following probability distributions,

$$p(a_j|A_j, \lambda) = \delta_{a_j, a_{j,\lambda}}, \tag{D.5a}$$

$$p(b_k|B_k, \lambda) = \delta_{b_k, b_{k,\lambda}}, \tag{D.5b}$$

$$p(\lambda) = p(a_1, a_2, b_1, b_2). \tag{D.5c}$$

By defining the probability distribution in (D.5), it is possible to define a LHV model with the marginal probability below,

$$\begin{aligned} p(a_j, b_k|A_j, B_k) &= \sum_{a_x|x\neq j, b_y|y\neq k} p(a_1, a_2, b_1, b_2) \\ &= \sum_{\lambda} p(\lambda)p(a_j|A_j, \lambda)p(b_k|B_k, \lambda). \end{aligned} \tag{D.6}$$

This completes the proof. □

Appendix E

General Bell's Inequality for N-qubits

In the paper [22] a general Bell's inequality was obtained. The general Bell's inequality is a sufficient and necessary condition for the correlation functions for a system of N-qubits measured from two possible settings for each qubit to be described by a local realistic model. We will present the derivation of the general Bell's inequality as in the paper.

Assuming that there are N observers trying to violate a single Bell's inequality. Each of the observers, say observer j, can choose two settings $\{\vec{n_1}, \vec{n}_2\}$, and there are only two possible measurement outcomes for each setting $a_j = +1$ or $a_j = -1$.

The correlation function for the N observers, as in equation (C.1), can be written as the expectation value of the product of their measurement outcomes given their respective settings,

$$E(\vec{k}) = \left\langle \prod_{j=1}^{N} a_j(\vec{n}_{k_j}) \right\rangle_{avg}, \tag{E.1}$$

where $k_j = 1, 2$ is the measurement setting number and $\vec{k}$ is the shorthand for $(k_1, ..., k_N)$.

It was shown that the following algebraic identity holds for pre-determined results:

$$\sum_{\vec{s}=\pm 1} S(\vec{s}) \prod_{j=1}^{N} [a_j(\vec{n}_1) + s_j a_j(\vec{n}_2)] = \pm 2^N, \tag{E.2}$$

where $s_j = \pm 1$, $\vec{s}$ is the shorthand for $(s_1, ..., s_N)$, and $S(\vec{s})$ is any arbitrary function of $\vec{s}$ such that its values are only ± 1. The proof for equation (E.2) can be seen that since $a_j(\vec{n}_1), a_j(\vec{n}_2) = \pm 1$, at least one product $\prod_{j=1}^{N} [a_j(\vec{n}_1) + s_j a_j(\vec{n}_2)] = \prod_{j=1}^{N} \pm 2 = \pm 2^N$ by setting $s_j = \frac{a_j(\vec{n}_1)}{a_j(\vec{n}_2)}$. However, the product does not vanish for only this combination of $\vec{s}$ because the product will have at least one zero term for any other combinations, and this completes the proof.

Averaging the experiment over many runs, equation (E.2) becomes

$$\left| \sum_{\vec{s}=\pm 1} S(\vec{s}) \sum_{\vec{k}=1,2} s_1^{k_1 - 1} ... s_N^{k_N - 1} E(\vec{k}) \right| \leqslant 2^N. \tag{E.3}$$

Since there are 2^{2^N} different functions of $S(\vec{s})$, this equation represents 2^{2^N} different Bell's inequalities.

For example, for $N = 2$, the CHSH inequality can be obtained by setting $S(s_1, s_2) = +1$ except for when $S(+1, -1) = -1$:

$$\begin{aligned} \sum_{s_1, s_2 = \pm 1} S(s_1, s_2) \sum_{k_1, k_2 = 1,2} & s_1^{k_1 - 1} s_2^{k_2 - 1} E(k_1, k_2) \\ =& E(1,1) + E(2,1) + E(1,2) + E(2,2) \\ & + E(1,1) - E(2,1) + E(1,2) - E(2,2) \\ & - [E(1,1) + E(2,1) - E(1,2) - E(2,2)] \\ & + E(1,1) - E(2,1) - E(1,2) + E(2,2) \\ =& 2[E(1,1) - E(2,1) + E(1,2) + E(2,2)], \end{aligned}$$

$$|E(1,1) - E(2,1) + E(1,2) + E(2,2)| \leqslant \frac{2^2}{2} = 2.$$

where the last equation is the CHSH inequality as in equation (C.9).

Equation E.4 is equivalent to

$$\sum_{\vec{s}=\pm 1} \left| \sum_{\vec{k}=1,2} s_1^{k_1-1} ... s_N^{k_N-1} E(\vec{k}) \right| \leqslant 2^N. \tag{E.4}$$

The equivalence can be seen by recognising that for any real number r_j, all possible combinations of $\left|\sum_j \pm r_j\right| \leqslant c$ hold if and only if $\sum_j |r_j| \leqslant c$ holds. Hence equation (E.4) is known as the general Bell's inequality.

Thus far only the necessary condition has been shown for local realistic model implying the general Bell's inequality. The converse is also true. The sufficient condition was shown to be true by constructing a local realistic model given that the general Bell's inequality holds.

Constructing the hidden probability for the condition $s_j = \frac{a_j(\vec{n}_1)}{a_j(\vec{n}_2)}$,

$$p(\vec{s}) = \frac{1}{2^N} \left| \sum_{\vec{k}=1,2} s_1^{k_1-1} ... s_N^{k_N-1} E(\vec{k}) \right|. \tag{E.5}$$

One can demand that $\prod_{j=1}^N a_j(\vec{n}_1)$ has the same sign as the expression in the modulus of equation (E.5). It can be shown that the correlation function (E^{LHV}) calculated from the marginal of $\prod_{j=1}^N a_j(\vec{n}_{k_j})$ over all possible $\vec{s}$ reduces back to the one obtained in the experiment, i.e.

$$E^{LHV}(\vec{k}) = \sum_{\vec{s}=\pm 1} p(\vec{s}) \prod_{j=1}^N a_j(\vec{n}_{k_j}) = E(\vec{k}). \tag{E.6}$$

For example, in the case of $N = 3$ and $\vec{k} = (1, 2, 1)$,

$$
\begin{aligned}
E^{LHV}(1,2,1) &= \sum_{s_1,s_2,s_3=\pm 1} p(s_1, s_2, s_3) \prod_{j=1}^{N} a_j(\vec{n}_{k_j}) \\
&= \sum_{s_1,s_2,s_3=\pm 1} \frac{1}{2^3} \left| \sum_{k_1,k_2,k_3=1,2} s_1^{k_1-1} s_2^{k_2-1} s_3^{k_3-1} E(k_1,k_2,k_3) \right| a_1(\vec{n}_1) a_2(\vec{n}_2) a_3(\vec{n}_1) \\
&= \sum_{s_1,s_2,s_3=\pm 1} \frac{1}{8} \left| \sum_{k_1,k_2,k_3=1,2} s_1^{k_1-1} s_2^{k_2-1} s_3^{k_3-1} E(k_1,k_2,k_3) \right| a_1(\vec{n}_1) \frac{a_2(\vec{n}_1)}{s_2} a_3(\vec{n}_1) \\
&= \sum_{s_1,s_2,s_3=\pm 1} \frac{1}{8} \sum_{k_1,k_2,k_3=1,2} s_1^{k_1-1} s_2^{k_2-2} s_3^{k_3-1} E(k_1,k_2,k_3) \\
&= \sum_{s_1,s_2,s_3=\pm 1} \frac{1}{8} [8E(1,2,1)] \\
&= E(1,2,1).
\end{aligned}
$$

In the case where the general Bell's inequality is not saturated and the sum of all the hidden probabilities is not unity, we can assign those "missing" probabilities to local realistic noise such that it does not affect the correlation function calculated. This ends the proof for the sufficiency condition. Hence it was proven that a local realistic model exist if and only if the general Bell's inequality in equation (E.4) holds.

The paper went on to show the condition for any arbitrary quantum state (pure or mixed) to satisfy equation (E.4).

An arbitrary quantum state of N-qubits can be represented as

$$
\rho = \frac{1}{2^N} \sum_{\mu_1,\ldots,\mu_N=0}^{3} T_{\mu_1 \ldots \mu_N} \sigma_{\mu_1}^{1} \otimes \ldots \otimes \sigma_{\mu_N}^{N}, \tag{E.7}
$$

where σ_0^j is the identity operator and $\sigma_{x_j}^j$ are the Pauli operators for the three orthogonal directions $x_j = 1, 2, 3$ in the Hilbert space of the jth qubit. The set of components $T_{\mu_1 \ldots \mu_N} = \mathrm{tr}(\rho.(\sigma_{\mu_1}^1 \otimes \ldots \otimes \sigma_{\mu_N}^N))$ corresponding to the three orthogonal Pauli operators forms the *correlation tensor*, $\hat{T}$.

Hence the correlation function corresponding to a N-qubit system is

$$\begin{aligned} E^{QM}(\vec{k}) &= \mathrm{tr}[\rho.(\vec{n}_{k_1}.\vec{\sigma} \otimes ... \otimes \vec{n}_{k_N}.\vec{\sigma})] \\ &= \sum_{x_1,...,x_N=1}^{3} T_{x_1...x_N} (\vec{n}_{k_1})_{x_1} ... (\vec{n}_{k_N})_{x_N}, \end{aligned} \tag{E.8}$$

where $(\vec{n}_{k_j})_{x_j}$ are the Cartesian components of the vector $\vec{n}_{k_j}$. This can be written in a more compact way as $\langle \hat{T}, \vec{n}_{k_1} \otimes ... \vec{n}_{k_N} \rangle$ where $\langle ..., ... \rangle$ denotes the scalar product in R^{3N}.

Putting correlation function for N-qubits system in equation (E.8) into the general Bell's inequality in equation (E.4), one obtain the condition for an arbitrary quantum state to have a local realistic model:

$$\sum_{\vec{s}=\pm 1} \left| \left\langle \hat{T}, \sum_{k_1=1}^{2} s_1^{k_1-1} \vec{n}_{k_1} \otimes ... \otimes \sum_{k_N=1}^{2} s_N^{k_N-1} \vec{n}_{k_N} \right\rangle \right| \leqslant 2^N. \tag{E.9}$$

For any pair of arbitrary unit vectors in R^3, $\{\vec{n}_1, \vec{n}_2\}$, the following properties hold: $\sum_{k_j=1}^{2} \vec{n}_{k_j} = 2c_1^j \vec{v}_1^j$ and $\sum_{k_j=1}^{2} (-1)^{k_j-1} \vec{n}_{k_j} = 2c_2^j \vec{v}_2^j$ where $(c_1^j)^2 + (c_2^j)^2 = 1$ and $\vec{v}_1^j.\vec{v}_2^j = 0$. Hence equation (E.9) can be simplified to

$$\sum_{x_1,...,x_N=1}^{2} \left| c_{x_1}^1 ... c_{x_N}^N \left\langle \hat{T}, \vec{v}_{x_1}^1 \otimes ... \otimes \vec{v}_{x_N}^N \right\rangle \right| \leqslant 1. \tag{E.10}$$

Equation (E.10) remains true for any local measurement settings of the N-qubits, hence we can write it as

$$\sum_{x_1,...,x_N=1}^{2} c_{x_1}^1 ... c_{x_N}^N \left| T_{x_1...x_N} \right| \leqslant 1, \tag{E.11}$$

where $T_{x_1...x_N}$ is a component of the correlation tensor in the new local coordinate system with $\{\vec{v}_1^j, \vec{v}_2^j\}$ among the new basic vectors. The two new basic vectors serve as unit vectors for, say, the local directions x and y. Therefore, the general Bell's inequality in equation (E.4) holds for an arbitrary quantum state of N-qubits if and only if equation (E.11) holds for any arbitrary set of local coordinate systems and any set of unit vectors $\vec{c}^j = (c_1^j, c_2^j)$.

The condition (E.11) is often hard to compute as it involves maximizing the correlation tensor over all local coordinates of the N observers to obtain the "largest plane" followed by a rotation in this plane. Applying the CauchySchwarz inequality to the inequality (E.11), a weaker condition is obtained:

$$\sum_{x_1,\ldots,x_N=1}^{2} T_{x_1\ldots x_N}^2 \leqslant 1. \tag{E.12}$$

If condition (E.12) holds for any local coordinate systems, then it would imply that the general Bell's inequality (E.4) holds.

Appendix F

Clique cover problem (MATLAB code)

File name: kf_complementarity.m

Description: Main function to calculate the bound from complementarity principle.

Author: Ng Kang Feng

```
function [min_clique_cover_number] = kf_complementarity(bell_particle_pos,
    element_no, permutation_no)
% This function calculates the bound from complementarity principle.
%
% Input:
% bell_particle_pos takes in cells of the position of the observers.
% For example, the square graph is {[1 2 3],[2 3 4],[3 4 1], [4 1 2]}
% element_no is the number of observers. The square graph has 4 observers.
% permutation_no is the number of orthogonal coordinates in the Bell
% parameters. It is usually equals to 2.
%
% Output:
```

```
% min_clique_cover_number outputs the bound from complementarity.



%We build the operators.
T = [];
for i = 1:length(bell_particle_pos)
T = [T;kf_correlation_tensor(bell_particle_pos{i}, element_no,
    permutation_no)];
end

%Calculate the bound from complementary.

%Prelimary--Create the anticommuting graph.
G = kf_commute_anticommute(T, permutation_no);

%Find the minimum clique cover by converting G to its complement Gbar.
%The steps below are to obtain the edge set of the complement graph E, and
%input the edge set into the ready written algorithm for finding the
%chromatic number.
[m,~] = size(G);
Gbar = G - tril(ones(m,m),-1);
[row,col] = find(Gbar == -1);
E = [row,col];
min_clique_cover_number = max(grColVerOld(E));
```

File name: kf_correlation_tensor.m

Description: A function to create the correlation tensors.

Author: Ng Kang Feng

```
function output = kf_correlation_tensor(bell_particle_pos, element_no,
    permutation_no)
% This function creates the needed correlation tensors.
%
% Input:
% bell_particle_pos takes in cells of the position of the observers.
% For example, the square graph is {[1 2 3],[2 3 4],[3 4 1], [4 1 2]}
% element_no is the number of observers. The square graph has 4 observers.
% permutation_no is the number of orthogonal coordinates in the Bell
% parameters. It is usually equals to 2.
%
% Output:
% Returns all the correlation tensors of the bell_particle_pos input.


m = length(bell_particle_pos);
vec = zeros(permutation_no^m, element_no);
combinations = combn(1:permutation_no,m);
vec(:,bell_particle_pos) = combinations;
output = vec;
end
```

File name: kf_commute_anticommute.m

Description: A function to create anticommuting graph.

Author: Ng Kang Feng

```
function output_graph = kf_commute_anticommute(T, permutation_no)
% This function creates the anticommuting graph.
%
```

```
% Input:
% T is the array of the operator.
% permutation_no is the number of orthogonal coordinates in the Bell
% parameters. It is usually equals to 2.
%
% Output:
% output_graph is the anticommuting graph.

[m,n] = size(T);
G = zeros(m,m);
C = nchoosek(1:permutation_no,2);
C = C(:,1).*C(:,2);

for i = 1:m
for j = i:m
v = T(i,:).*T(j,:);
counter = 0;
for l = 1:nchoosek(permutation_no,2)
counter = counter + sum(v == C(l));
end
if mod(counter,2) == 1
G(i,j) = 1;
end
end
output_graph = G + G';
end
```

File name: combn.m

Description: A function to create all combinations of a certain set.

Author: Jos (10584)

URL: `http://www.mathworks.com/matlabcentral/fileexchange/7147-combn--4-3-/content//combn.m`

```
function [M,IND] = combn(V,N)
% COMBN - all combinations of elements
%   M = COMBN(V,N) returns all combinations of N elements of the elements
    in
%   vector V. M has the size (length(V).^N)-by-N.
%
%   [M,I] = COMBN(V,N) also returns the index matrix I so that M = V(I).
%
%   V can be an array of numbers, cells or strings.
%
%   Example:
%     M = COMBN([0 1],3) returns the 8-by-3 matrix:
%       0     0     0
%       0     0     1
%       0     1     0
%       0     1     1
%       ...
%       1     1     1
%
%   All elements in V are regarded as unique, so M = COMBN([2 2],3) returns
%   a 8-by-3 matrix with all elements equal to 2.
%
%   NB Matrix sizes increases exponentially at rate (n^N)*N. For larger
%   values of n and N, one could loop over the output of COMBNSUB
```

```
%   retrieving one or more rows of the output at a single time.
%
%   See also PERMS, NCHOOSEK
%        and COMBNSUB, ALLCOMB, and PERMPOS on the File Exchange

% tested in Matlab R13, R14, 2010b
% version 4.3 (apr 2013)
% (c) Jos van der Geest
% email: jos@jasen.nl

% History
% 1.1 updated help text
% 2.0 new faster algorithm
% 3.0 (aug 2006) implemented very fast algorithm
% 3.1 (may 2007) Improved algorithm Roger Stafford pointed out that for
    some values, the floor
% operation on floating points, according to the IEEE 754 standard, could
    return
% erroneous values. His excellent solution was to add (1/2) to the values
% of A.
% 3.2 (may 2007) changed help and error messages slightly
% 4.0 (may 2008) again a faster implementation, based on ALLCOMB, suggested
     on the
%    newsgroup comp.soft-sys.matlab on May 7th 2008 by "Helper". It was
%    pointed out that COMBN(V,N) equals ALLCOMB(V,V,V...) (V repeated N
%    times), ALLCMOB being faster. Actually version 4 is an improvement
%    over version 1 ...
% 4.1 (jan 2010) removed call to FLIPLR, using refered indexing N:-1:1
%    (is faster, suggestion of Jan Simon, jan 2010), removed REPMAT, and
```

```
%    let NDGRID handle this
% 4.2 (apr 2011) corrrectly return a column vector for N = 1 (error pointed
%     out by Wilson).
% 4.3 (apr 2013) make a reference to COMBNSUB

error(nargchk(2,2,nargin)) ;

if isempty(V) || N == 0,
M = [] ;
IND = [] ;
elseif fix(N) ~= N || N < 1 || numel(N) ~= 1 ;
error('combn:negativeN','Second argument should be a positive integer') ;
elseif N==1,
% return column vectors
M = V(:) ;
IND = (1:numel(V)).' ;
else
% speed depends on the number of output arguments
if nargout<2,
M = local_allcomb(V,N) ;
else
% indices requested
IND = local_allcomb(1:numel(V),N) ;
M = V(IND) ;
end
end

% LOCAL FUNCTIONS
```

```
function Y = local_allcomb(X,N)
% See ALLCOMB, available on the File Exchange
if N>1
% create a list of all possible combinations of N elements
[Y{N:-1:1}] = ndgrid(X) ;
% concatenate into one matrix, reshape into 2D and flip columns
Y = reshape(cat(N+1,Y{:}),[],N) ;
else
% no combinations have to be made
Y = X(:) ;
end

% =========================================================================
% Previous algorithms



% Version 3.2
%     % COMBN is very fast using a single matrix multiplication, without any
%       explicit for-loops.
%     nV = numel(V) ;
%     % use a math trick
%     A = [0:nV^N-1]+(1/2) ;
%     B = [nV.^(1-N:0)] ;
%     IND = rem(floor((A(:) * B(:)')),nV) + 1 ;
%     M = V(IND) ;

% Version 2.0
%     for i = N:-1:1
%         X = repmat(1:nV,nV^(N-i),nV^(i-1));
```

```
%        IND(:,i) = X(:);
%    end
%    M = V(IND) ;

% Version 1.0
%    nV = numel(V) ;
%    % don waste space, if only one output is requested
%    [IND{1:N}] = ndgrid(1:nV) ;
%    IND = fliplr(reshape(cat(ndims(IND{1}),IND{:}),[],N)) ;
%    M = V(IND) ;



% Combinations using for-loops
% can be implemented in C or VB
% nv = length(V) ;
% C = zeros(nv^N,N) ; % declaration
% for ii=1:N,
%    cc = 1 ;
%    for jj=1:(nv^(ii-1)),
%        for kk=1:nv,
%            for mm=1:(nv^(N-ii)),
%                C(cc,ii) = V(kk) ;
%                cc = cc + 1 ;
%            end
%        end
%    end
% end
```

File name: grColVerOld.m

Description: A function to find the chromatic number of a graph.

Author: Sergii Iglin

URL: http://www.mathworks.com/matlabcentral/fileexchange/4266-grtheory-graph-theory-toolbox/content//grColVerOld.m

```
function nCol=grColVerOld(E)
% function nCol=grColVer(E) solve the color graph problem
% for vertexes of the graph.
% Input parameter:
%   E(m,2) - the edges of graph;
%     1st and 2nd elements of each row is numbers of vertexes;
%     m - number of edges.
% Output parameter:
%   nCol(n,1) - the list of the colors of vertexes.
% Uses the sequential deleting of the maximal stable sets.
% Required the Optimization Toolbox v.3.0.1 or over.
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% ============= Input data validation ==================
if nargin<1,
error('There are no input data!')
end
[m,n,E] = grValidation(E); % E data validation
E=sort(E(:,1:2)')'; % each row in ascending order
E=unique(E,'rows'); % we delete multiple edges
```

```
E=E(setdiff([1:size(E,1)]',find((E(:,1)==E(:,2)))),:); % we delete loops
nCol=zeros(n,1); % initial value
% ============= Main cycle with MaxStabSet deleting ====
while any(nCol==0),
nv=find(nCol==0); % uncolored vertexes
E1=E(find(ismember(E(:,1),nv)&ismember(E(:,2),nv)),:); % it's edges
if isempty(E1),
nCol(find(nCol==0))=max(nCol)+1; % the last color
break;
end
nvs=unique(E1(:)); % all vertexes
for kk=1:length(nvs),
E1(find(E1==nvs(kk)))=kk;
end
nMS=grMaxStabSet(E1); % the maximal stable set
nCol(nvs(nMS))=max(nCol)+1; % the next color
end
return
```

File name: grMaxStabSet.m

Description: A function used in grColVerOld.m.

Author: Sergii Iglin

URL: http://www.mathworks.com/matlabcentral/fileexchange/4266-grtheory-graph-theory-toolbox/content//grMaxStabSet.m

```
function nMS=grMaxStabSet(E,d)
% Function nMS=grMaxStabSet(E,d) solve the maximal stable set problem.
% Input parameters:
%   E(m,2) - the edges of graph;
```

```
%    1st and 2nd elements of each row is numbers of vertexes;
%    m - number of edges.
%  d(n) (optional) - the weights of vertexes,
%    n - number of vertexes.
%    If we have only 1st parameter E, then all d=1.
% Output parameter:
%  nMS - the list of the numbers of vertexes included
%    in the maximal (weighted) stable set.
% Uses the reduction to integer LP-problem.
% Required the Optimization Toolbox v.3.0.1 or over.
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% ============= Input data validation ==================
if nargin<1,
error('There are no input data!')
end
[m,n,E] = grValidation(E); % E data validation
if nargin<2, % we may only 1st parameter
d=ones(n,1); % all weights =1
else
d=d(:); % reshape to vector-column
if length(d)<n, % the poor length
error('The length of the vector d is poor!')
else
n=length(d); % Number of Vertexes
end
end
```

```
% ============= Parameters of integer LP problem ==========
A=zeros(n,m); % for incidence matrix
A(E(:,1:2)+repmat(([1:m]'-1)*n,1,2))=1; % we fill the incidence matrix
options=optimset('bintprog'); % the default options
options.Display='off'; % we change the output

% ============= We solve the MILP problem ==========
xmin=bintprog(-d,A',ones(m,1),[],[],[],options);
nMS=find(round(xmin)); % the answer - numbers of vertexes
return
```

File name: grValidation.m

Description: A function used in grColVerOld.m.

Author: Sergii Iglin

URL: http://www.mathworks.com/matlabcentral/fileexchange/4266-grtheory-graph-theory-toolbox/content//grValidation.m

```
function [m,n,newE] = grValidation(E);
% The validation of array E - auxiliary function for GrTheory Toolbox.
% Author: Sergii Iglin
% e-mail: siglin@yandex.ru
% personal page: http://iglin.exponenta.ru

if ~isnumeric(E),
error('The array E must be numeric!')
end
if ~isreal(E),
error('The array E must be real!')
```

```
end
se=size(E); % size of array E
if length(se)~=2,
error('The array E must be 2D!')
end
if (se(2)<2),
error('The array E must have 2 or 3 columns!'),
end
if ~all(all(E(:,1:2)>0)),
error('1st and 2nd columns of the array E must be positive!')
end
if ~all(all((E(:,1:2)==round(E(:,1:2))))),
error('1st and 2nd columns of the array E must be integer!')
end
m=se(1);
if se(2)<3, % not set the weight
E(:,3)=1; % all weights =1
end
newE=E(:,1:3);
n=max(max(newE(:,1:2))); % number of vertexes
return
```

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